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Physics Procedia 57 (2014) 99 – 103

Physics Procedia

27th Annual CSP Workshops on "Recent Developments in Computer Simulation Studies in Condensed Matter Physics", CSP 2014

The Inverse Ising Problem

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Abstract

The inverse Ising problem consists of taking a set of Ising configurations generated with unknown interaction parameters, and determining reliable estimates for the values of those interaction parameters. The problem first arose in connection with the Monte Carlo renormalization group, and was solved thirty years ago. Recently, there has been renewed interest in the inverse Ising problem due to biological applications. The original solution seems to have been forgotten, as it was rediscovered in a different representation by Aurell and Ekeberg in 2012. In this paper we modify the earlier equations to solve problems that are not translationally invariant.

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Keywords: Monte Carlo, Ising, Inverse

1. Introduction

A common use of Markov Chain Monte Carlo computer simulations (MCMC, or simply MC) is to generate configurations with the Boltzmann probability distribution for a model Hamiltonian describing the interactions between particles or spins. The object of such simulations is to obtain the thermodynamic properties of the model, and many procedures for the efficient implementation of such computations have been developed (Landau and Binder, 2009).

The inverse problem has arisen in various fields, in which experiments have led to the question of how correlations in experimental data can be understood in terms of effective underlying interactions (Aurell and Ekeberg, 2012). This, in turn, has led to the question of how to invert the usual Monte Carlo simulation process, which is the subject of this paper. In particular, we are concerned with the inverse Ising problem, in which a set of configurations of spins on a lattice with values $\sigma_j = \pm 1$ is given – either from experiment or model calculations – and the object is to reconstruct the effective Hamiltonian that corresponds to these configurations.

The inverse Ising problem had first arisen in the 1970's and 1980's, during the development of the Monte Carlo renormalization group analysis of critical phenomena. Equations for determining critical exponents from MC computer simulations were found first (Ma, 1976; Swendsen, 1979). However, those equations did not provide estimates of the renormalized Hamiltonians or the locations of fixed points. The problem of determining the renormalized coupling parameters was solved by (Swendsen, 1984a,b,c).

In 2012, the earlier solution was rediscovered in a different representation (Aurell and Ekeberg, 2012). Both representations have advantages. The Aurell and Ekeberg version of the solution uses pseudolikelihood maximization, which emphasizes the connection to probability theory. The earlier representation makes the connection to the cor-

Peer-review under responsibility of The Organizing Committee of CSP 2014 conference
doi:10.1016/j.phpro.2014.08.140

relation functions obtained from the configurations more apparent, and clarifies the distinction between fitting the correlation functions and inferring the effective coupling constants.

Recent theoretical work in the inverse Ising problem has concentrated on determining the coupling constants from configurations of spins generated from the Sherrington-Kirkpatrick (SK) model of a spin glass (Kirkpatrick and Sherrington, 1975). This model contains N Ising spins governed by a Hamiltonian of the form where the couplings $J_{j,k}$ are drawn from a quenched Gaussian distribution of width $1/\sqrt{N}$. The local magnetic fields b_j can also be given independent quenched values, but they are frequently set to zero for simplicity in studying the efficiency of proposed algorithms for the solution of this problem. We will usually express our calculations and results in terms of the dimensionless coupling constants $K_{j,k} = \beta J_{j,k}$ and $h_j = \beta b_j$, where $\beta = 1/k_B T$, and k_B is Boltzmann's constant.

In the next section, we will give a simplified version of the 1984 solution. Since the SK model is limited to pairwise interactions and local fields, this simplified version is sufficient for the present discussion.

In subsequent sections, we will discuss how the limited information contained in correlation functions obtained from incomplete sampling limit the accuracy with which it is possible to infer the values of the coupling constants. There is no significant limit on the accuracy with which the correlation functions can be fit.

2. The inverse Ising equations for the SK model

The key observation needed to derive equations for the coupling constants comes in the form of an identity due to Callen (Callen, 1963). For a configuration σ, the effective field on spin σ_ℓ is

$$f_\ell(\sigma) = \sum_j K_{\ell,j}\sigma_j + h_\ell. \tag{1}$$

Callen demonstrated that the local magnetization is given by two distinct expressions.

$$\langle \sigma_\ell \rangle = \langle \tanh(f_\ell(\sigma)) \rangle \tag{2}$$

Similarly, each correlation function is given by three distinct expressions.

$$\langle \sigma_j \sigma_k \rangle = \langle \tanh(f_j(\sigma))\,\sigma_k \rangle = \langle \sigma_j \, \tanh(f_k(\sigma)) \rangle \tag{3}$$

Naturally, Eqs. (2) and (3) are only exact for complete data ($N_{\rm MC} = \infty$) and the exact values of the coupling constants are used. However, these equations do allow us to find *effective* coupling constants that fit the empirical correlation functions to arbitrary accuracy.

For clarity, denote the values of the correlation functions obtained from direct averages over the given set of configurations by $m_j^* = \langle \sigma_j \rangle_{\rm MC}$ and $c_{j,k}^* = \langle \sigma_j \sigma_k \rangle_{\rm MC}$. The values of coupling constants that would exactly reproduce these functions in Eqs. (2) and (3) will be denoted as $\{K_{j,k}^*\}$ and $\{h_j^*\}$. These are the target values of our computation, since they would give a complete representation of the information contained in the measured correlation functions.

The problem of determining the effective coupling constants breaks up into N separate calculations (Aurell and Ekeberg, 2012), one for each of the subsets of interactions that connect to an individual 'central' spin that we will denote as ℓ. The neighbors of ℓ will be denoted by $\ell + \delta$. The Hamiltonian for the cluster of spins connected to σ_ℓ is then

$$H_\ell = \sigma_\ell \left[\sum_\delta K_{\ell,\ell+\delta}\,\sigma_{\ell+\delta} + h_\ell \right], \tag{4}$$

and the Callen equations are

$$m_\ell^* = \left\langle \tanh\left(h_\ell + \sum_\delta K_{\ell,\ell+\delta}\sigma_{j+\delta} \right) \right\rangle \tag{5}$$

and

$$c_{\ell,\ell+\delta}^* = \left\langle \sigma_{\ell+\delta} \tanh\left(h_\ell + \sum_\delta K_{\ell,\ell+\delta}\sigma_{\ell+\delta} \right) \right\rangle. \tag{6}$$

Eqs. (5) and (6) correspond to Eq. (14) in Ref. (Swendsen, 1984a), and Eq. (4) in Ref. (Aurell and Ekeberg, 2012).

To obtain an iterative solution to these equations, we also need all derivatives with respect to the coupling parameters. Taking the derivative of Eq. (5) with respect to h_ℓ gives

$$\frac{\partial m_\ell^*}{\partial h_\ell} = \left\langle \mathrm{sech}^2 \left(h_\ell + \sum_\delta K_{\ell,\ell+\delta}\sigma_{\ell+\delta} \right) \right\rangle, \tag{7}$$

and the derivative with respect to $K_{\ell,\ell+\delta}$

$$\frac{\partial m_\ell^*}{\partial K_{\ell,\ell+\delta}} = \left\langle \sigma_{\ell+\delta}\, \mathrm{sech}^2 \left(h_\ell + \sum_\delta K_{\ell,\ell+\delta}\sigma_{\ell+\delta} \right) \right\rangle, \tag{8}$$

Similarly, we have the derivative of $c^*_{\ell,\ell+\delta}$ with respect to h_ℓ

$$\frac{\partial c^*_{\ell,\ell+\delta}}{\partial h_\ell} = \left\langle \sigma_{\ell+\delta}\, \mathrm{sech}^2 \left(h_\ell + \sum_\delta K_{\ell,\ell+\delta}\sigma_{\ell+\delta} \right) \right\rangle, \tag{9}$$

and the derivative with respect to $K_{\ell,\ell+\delta'}$, where $\ell + \delta'$ also runs over the neighbors of the central site ℓ.

$$\frac{\partial c^*_{\ell,\ell+\delta}}{\partial K_{\ell,\ell+\delta'}} = \left\langle \sigma_{\ell+\delta}\, \sigma_{\ell+\delta'}\, \mathrm{sech}^2 \left(h_\ell + \sum_\delta K_{\ell,\ell+\delta}\sigma_{\ell+\delta} \right) \right\rangle. \tag{10}$$

Eqs. (7) through (10) correspond to Eq. (15) in Ref. (Swendsen, 1984a), and Eq. (7) in Ref. (Aurell and Ekeberg, 2012).

Since $\mathrm{sech}^2(\theta) > 0$, the maximum magnitude of the derivatives is found in the diagonal terms, which all have the same value. The off-diagonal terms can have cancellations between positive and negative contributions, so they are usually smaller.

The iterative equations are

$$m_\ell^* - m_\ell = \frac{\partial m_\ell^*}{\partial h_\ell}\delta h_\ell + \sum_\delta \frac{\partial m_\ell^*}{\partial K_{\ell,\ell+\delta}}\delta K_{\ell,\ell+\delta} \tag{11}$$

and

$$c^*_{\ell,\ell+\delta} - c_{\ell,\ell+\delta} = \frac{\partial c^*_{\ell,\ell+\delta}}{\partial h_\ell}\delta h_\ell + \sum_{\delta'} \frac{\partial c^*_{\ell,\ell+\delta}}{\partial K_{\ell,\ell+\delta'}}\delta K_{\ell,\ell+\delta'} \tag{12}$$

After solving the linearized equations for δm_ℓ and $\delta c_{\ell,\ell+\delta}$, the new estimates for the coupling parameters should be used to recompute the derivatives and repeat the solution of the linearized equations. This process of iteration should converge to the best estimate of the couplings connected to the spin at site ℓ.

3. Limits on the accuracy of the solution

We must make a distinction between the accuracy with which we can fit the measured correlation functions and the accuracy with which we can reproduce the original coupling constants. To clarify this distinction, consider the very simple case of a single spin in a magnetic field, h.

$$H = -b\,\sigma \tag{13}$$

The expectation value of the magnetization is well known to be

$$\langle \sigma \rangle = \tanh(\beta b), \tag{14}$$

where $\beta = 1/k_B T$, k_B is Boltzmann's constant, and T is temperature.

Assume that we have an estimate of the magnetization from a Monte Carlo simulation of N_{MC} independent values of σ.

$$\langle\sigma\rangle_{\mathrm{MC}} = \frac{1}{N_{\mathrm{MC}}} \sum_{t=1}^{N_{\mathrm{MC}}} \sigma(t), \tag{15}$$

where $t = 1, \ldots, N_{\mathrm{MC}}$ labels the Monte Carlo time steps.

From Eq. (14), we can easily find an estimate $b_{\mathrm{eff}} \approx b$ from $\langle\sigma\rangle_{\mathrm{MC}}$.

$$b_{\mathrm{eff}} = k_B T \tanh^{-1}\left(\langle\sigma\rangle_{\mathrm{MC}}\right) \tag{16}$$

We can, of course, solve Eq. (16) to arbitrary accuracy. However, the resultant b_{eff} will not be exactly equal to the true value of h because of the incomplete MC sampling that was restricted to a finite number of configurations.

We can estimate the error δb_{eff} as

$$\delta b_{\mathrm{eff}} = k_B T \frac{\cosh(\beta h)}{\sqrt{N_{\mathrm{MC}}}}, \tag{17}$$

which gives a minimum error of $\delta b_{\mathrm{min}} = k_B T / \sqrt{N_{\mathrm{MC}}}$.

4. Numerical solution of the inverse Ising equations for spin-glass models

To illustrate the numerical solution of the inverse Ising problem without translational invariance, we have simulated two spin-glass models on two-dimensional lattices, and then inferred the values of the local magnetic fields and coupling constants from the equations given above in Section 2. The first example had quenched pairwise coupling constants of $+1$ and -1 with equal probability, with all local fields set equal to zero. The lattice size was 32×32, and the temperature was set to be $T = 1.0$. As shown by the histograms in Fig. 1, the estimates for the coupling constants are tightly clustered around the correct values of ± 1, while the estimates of the local magnetic fields are tightly clustered around zero.

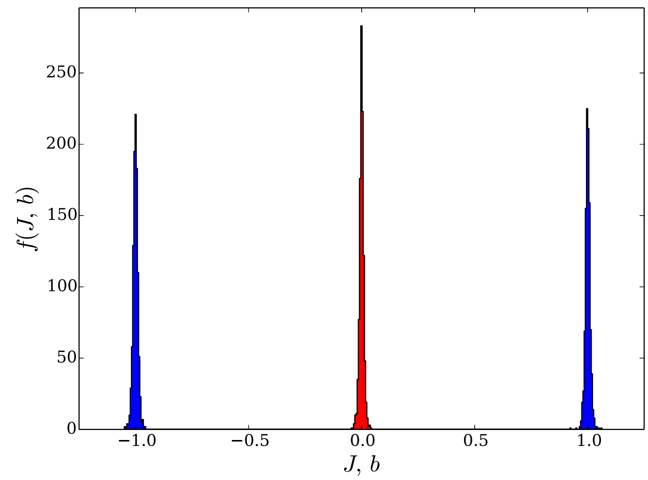

Fig. 1. Histograms of the estimated coupling constants, $F(J)$, and local magnetic fields, $F(b)$, for a 32×32 Ising model with values of $J_{j,k}$ chosen randomly to be ± 1 and the local magnetic fields set to zero, $b_j = 0$. The input data from the MC simulation contained 2.5×10^5 configurations. The red peak around $b = 0$ is entirely from estimates of local magnetic fields, and the blue peaks around $j = \pm 1$ are entirely from two-spin interactions.

For the second example, we chose both the local magnetic fields and the pairwise coupling constants from a uniform distribution between -1 and $+1$, and computed the errors for a temperature range from $T = 0.75$ to $T = 1.5$.

Fig. 2, shows the errors in reconstructing the coupling constants and local fields as functions of temperature. As the temperature is lowered, errors increase due to both the cosh(βh) factor in Eq. (17) and, more importantly, the increasingly strong correlations between the spins. The larger errors at low temperatures reflect the well-known phenomenon that spin glasses become trapped in deep free-energy minima. This makes sampling inefficient and limits the information contained in samples generated by computer simulations. It should be emphasized, that the errors are due to limitations in the information contained in the correlation functions. The errors do not represent a limitation of our method for inferring values of the coupling constants.

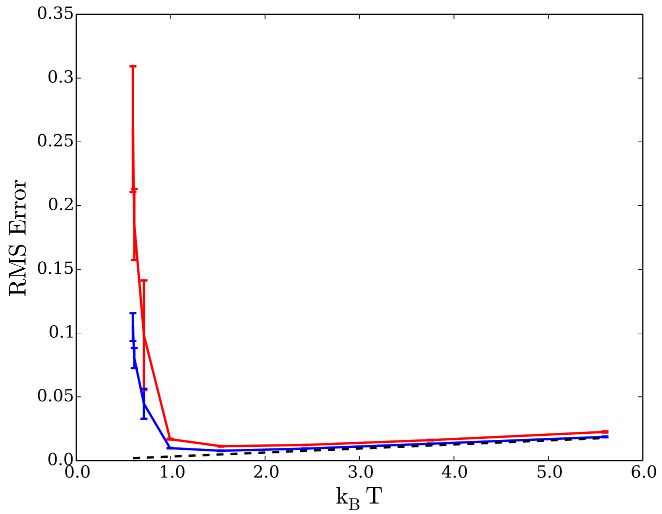

Fig. 2. Plot of the errors in estimated coupling constants an Ising spin-glass on a 32 × 32 lattice with both nearest-neighbor interactions and local magnetic fields were generated from a uniform distribution in the range $[-1, 1]$. The input data from the MC simulation contained 10^5 configurations. The errors in the estimated local magnetic fields (red) are larger than those for the two-spin interactions (blue). This is a general feature that we have seen for a variety of models we have investigated.

5. Future work

The equations derived in the original 1984 solution were written for translationally invariant problems, but were explicitly extended to multi-spin interactions. For simplicity, we have restricted the equations in this paper to local magnetic fields and two-spin interactions. However, the inclusion of multi-spin interactions is straightforward, and will be reported elsewhere (Albert and Swendsen, 2014).

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