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Bethe–Peierls approximation and the inverse Ising problem

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Abstract. We apply the Bethe–Peierls approximation to the inverse Ising problem and show how the linear response relation leads to a simple method for reconstructing couplings and fields of the Ising model. This reconstruction is exact on tree graphs, yet its computational expense is comparable to those of other mean-field methods. We compare the performance of this method to the independent-pair, naive mean-field, and Thouless–Anderson–Palmer approximations, the Sessak–Monasson expansion, and susceptibility propagation on the Cayley tree, SK model and random graph with fixed connectivity. At low temperatures, Bethe reconstruction outperforms all of these methods, while at high temperatures it is comparable to the best method available so far (the Sessak–Monasson method). The relationship between Bethe reconstruction and other mean-field methods is discussed.

Keywords: data mining (theory), network reconstruction, learning theory, statistical inference

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The enormous and ongoing growth of data in molecular biology has led to a surge of interest in inverse problems. Examples include the reconstruction of gene regulatory networks from expression levels [1], the identification of neural interactions from neural spike recordings [2], and the prediction of protein–protein interactions from the evolutionary correlation between amino acids [3]. The paradigm for such inverse problems is the inverse Ising problem, where the parameters of the Ising model Hamiltonian (couplings and fields) are to be inferred from a set of spin configurations drawn independently from the equilibrium measure. The goal is to use correlations observed between spins to infer the underlying, unknown couplings and fields. This problem is intrinsically hard, as pairs of spins can exhibit correlations without interacting directly with each other.

In this note, we consider the inverse Ising model at the level of the Bethe–Peierls approximation (BP) and show how the linear response approach [4]–[6] leads to a reconstruction of the Ising model that is efficient and straightforward, and outperforms currently available mean-field-like methods on benchmarks for strong couplings (and does as well as they do at weak couplings).

Consider the Boltzmann measure

$$p[\mathbf{s}] = \frac{1}{Z} e^{-H[\mathbf{s}]} \quad (1)$$

of the Ising model with $H[\mathbf{s}] = -\sum_i h_i s_i - \sum_{(ij)} J_{ij} s_i s_j$, specifying the statistical weight of a configuration $\mathbf{s} = (s_1, s_2, \dots, s_N)$ given couplings J_{ij} and local fields h_i (at inverse temperature $\beta = 1$), where Z is the partition function. The indices (ij) run over all pairwise interactions. The inverse Ising problem is then to recover the couplings and fields from a given set of M spin configurations $D = \{\mathbf{s}^1, \mathbf{s}^2, \dots, \mathbf{s}^M\}$ drawn independently from (1). The log-likelihood of couplings and fields given such a set of observations, normalized by M , is

$$L(\{s_i^\mu\}|\{h_i, J_{ij}\}) = -\ln Z[\{h_i, J_{ij}\}] + \sum_i h_i \frac{1}{M} \sum_\mu s_i^\mu + \sum_{(ij)} J_{ij} \frac{1}{M} \sum_\mu s_i^\mu s_j^\mu. \quad (2)$$

Maximizing the log-likelihood with respect to the Ising model parameters J_{ij} and h_i leads to

$$m_i(\{h_i, J_{ij}\}) = m_i^D, \quad C_{ij}(\{h_i, J_{ij}\}) = C_{ij}^D, \quad (3)$$

where $m_i = \langle s_i \rangle$ and $C_{ij} = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$ are the magnetizations and connected correlations under the Boltzmann distribution (1). The right-hand sides are the corresponding quantities estimated from data, $m_i^D = (1/M) \sum_\mu s_i^\mu$ and $C_{ij}^D = (1/M) \sum_\mu s_i^\mu s_j^\mu - m_i^D m_j^D$ [7].

Many different approaches to finding the couplings J_{ij} and fields h_i by maximizing the log-likelihood (2) or by directly solving the self-consistent equations (3) have been taken, including those based on gradient descent with Monte Carlo simulation [7], independent-pair approximation (IP) [8], naive mean-field (MF) [4], Thouless–Anderson–Palmer approximation (TAP) [4, 9], Sessak–Monasson expansion (SM) [10], susceptibility propagation (SusP) [11, 12] and more recently an adaptive cluster expansion [13] and pseudo-likelihood maximization [14, 15]. The canonical way to use a mean-field approximation for the inverse problem is to calculate the correlations through the linear

response of the magnetizations m_i to changes of the local fields h_i to yield the connected correlations and solve for the couplings. In the same way, our approach is based on the Bethe–Peierls approximation [16] combined with the linear response relation.

We begin by deriving the connected correlation for a system of spins in a tree graph, where the Boltzmann distribution (1) can be written exactly in terms of the Bethe ansatz, that is the combination of the one-point marginals b_i at the spins and the two-point marginals b_{ij} at the bonds:

$$p_{\text{BP}}[\mathbf{s}] = \prod_i b_i(s_i)^{1-z_i} \prod_{(i,j)} b_{ij}(s_i, s_j), \quad (4)$$

where z_i is the number of non-zero bonds connected to spin i [16]–[20]. The marginals b_i and b_{ij} , which are still unknown, can be parameterized with local magnetizations m_i and correlation parameters \bar{C}_{ij} as

$$b_i(s_i) = \frac{1}{2}(1 + m_i s_i), \quad b_{ij}(s_i, s_j) = \frac{1}{4}[(1 + m_i s_i)(1 + m_j s_j) + \bar{C}_{ij} s_i s_j], \quad (5)$$

with constraints

$$-1 \leq m_i \leq +1, \quad -1 + |m_i + m_j| - m_i m_j \leq \bar{C}_{ij} \leq +1 - |m_i - m_j| - m_i m_j. \quad (6)$$

Instead of *single spins* coupled to effective fields in naive mean-field theory, the Bethe ansatz is based on *bonds*. It is thus a natural approximation to take in the context of the inverse problem, where it is bonds that are to be determined, not the statistics of spins.

The self-consistent equations for the parameters m_i and \bar{C}_{ij} describing the statistics of spin pairs in equation (5) can be found by minimizing the Kullback–Leibler divergence \mathcal{D} between the Bethe ansatz (4) and the Boltzmann measure (1), $\mathcal{D}(p_{\text{BP}}[\mathbf{s}], p[\mathbf{s}]) = \sum_{\mathbf{s}} p_{\text{BP}}[\mathbf{s}] \ln(p_{\text{BP}}[\mathbf{s}]/p[\mathbf{s}])$, giving

$$h_i + \sum_{j \in \partial i} J_{ij} m_j = (1 - z_i) \text{arctanh}(m_i) + \sum_{j \in \partial i} \sum_{s_i, s_j} \frac{s_i + m_j s_i s_j}{4} \ln \frac{(1 + m_i s_i)(1 + m_j s_j) + \bar{C}_{ij} s_i s_j}{4}, \quad (7)$$

$$J_{ij} = \sum_{s_i, s_j} \frac{s_i s_j}{4} \ln \frac{(1 + m_i s_i)(1 + m_j s_j) + \bar{C}_{ij} s_i s_j}{4}, \quad (8)$$

where ∂i stands for the boundary set containing all spins that are connected to spin i by a bond.

The self-consistent equation (8) is quadratic in \bar{C}_{ij} , but only one of its solutions is compatible with the constraint (6), which is

$$\bar{C}_{ij} = \frac{(1 - m_i^2 - m_j^2)t_{ij} + 2m_i m_j}{1 + \sqrt{D_{ij}}} - m_i m_j, \quad (9)$$

where $D_{ij} = 1 - 2m_i m_j t_{ij} - (1 - m_i^2 - m_j^2)t_{ij}^2$ and $t_{ij} = \tanh(2J_{ij})$.

The correlation parameters \bar{C}_{ij} give the connected correlation for pairs of spins that interact with each other in the tree. To find the connected correlation C_{ij} between *any pair* of spins, we follow a route based on the linear response relation [4, 5, 20].

Differentiating the self-consistent equations (7) and (9) with respect to the fields h_i yields a set of equations for the susceptibilities $\partial m_i / \partial h_j$. The general linear response relation $C_{ij} = \partial m_i / \partial h_j$ then directly gives the connected correlations, for which we obtain

$$(C^{-1})_{ij} = -J_{ij} + \tilde{J}_{ij} + \frac{\bar{C}_{ij}}{(\bar{C}_{ij})^2 - (1 - m_i^2)(1 - m_j^2)}, \quad (i \neq j), \quad (10)$$

$$(C^{-1})_{ii} = \frac{1 - z_i}{1 - m_i^2} - \sum_{j \in \partial i} \frac{1 - m_j^2}{(\bar{C}_{ij})^2 - (1 - m_i^2)(1 - m_j^2)}, \quad (11)$$

with

$$\tilde{J}_{ij} = \frac{1}{4} \ln \left\{ \frac{[(1 + m_i)(1 + m_j) + \bar{C}_{ij}][(1 - m_i)(1 - m_j) + \bar{C}_{ij}]}{[(1 + m_i)(1 - m_j) - \bar{C}_{ij}][(1 - m_i)(1 + m_j) - \bar{C}_{ij}]} \right\}, \quad (12)$$

where the coupling matrix J_{ij} was extended to every pair of spins such that $J_{ij} = 0$ if i and j are not connected by a bond.

Note that the first two terms in the right-hand side of equation (10) cancel exactly due to (8); we however keep them to relate the expression to the Sessak–Monasson expansion later on.

An equivalent version of equations (10)–(12) was derived by Welling and Teh in the context of the forward problem [5], and was used to estimate the data evidence in Bayesian inference [21]. These equations can be also used to estimate the couplings and local fields in the inverse Ising problem. To do so, we first assume a fully connected model without self-interactions. It follows that $z_i = N - 1$, where N is the number of spins. The Bethe ansatz, together with the equations (7), (8), (10) and (11), is exact only in tree graphs; using it as an approximation in loopy graphs is usually referred to as Bethe–Peierls approximation. In loopy graphs, the correlation between interacting spins estimated using the linear response relation (10) is different from the correlation parameter (9), which is, in general, of lower accuracy [6]. In equation (10), we identify the magnetizations m_i and the connected correlations C_{ij} with the values m_i^D and C_{ij}^D estimated from data. Inserting the solution (9) for the correlation parameters \bar{C}_{ij} , equation (10) is solved for the couplings J_{ij} . To calculate the local fields h_i , the solutions J_{ij} are fed into the self-consistent equation (7). Its solution in closed form completes the Bethe reconstruction.

The Bethe–Peierls approximation is related to a number of previous approaches. Expanding equation (10) to first and second order in J_{ij} recovers the naive mean-field and TAP reconstructions, respectively. Calculating the couplings and local fields using the self-consistent equations (7) and (8) with $m_i = m_i^D$ and $\bar{C}_{ij} = C_{ij}^D$ estimated from data leads to the independent-pair approximation [8]. On the other hand, inserting the estimated values m_i^D and C_{ij}^D into the places of m_i and C_{ij} as well as \bar{C}_{ij} in equation (10) (without using the solution (9) for \bar{C}_{ij}), one obtains the Sessak–Monasson reconstruction [8, 10]. And lastly, since the extrema of Bethe–Peierls free energy are the fixed points of belief propagation [22], susceptibility propagation is expected to have a fixed point at the solution of the Bethe reconstruction.

Interestingly, for a tree at zero field, the magnetizations m_i are zero for finite system, and equations (10) and (11) take on a particularly simple form: $(C^{-1})_{ij} = -\sinh(J_{ij})\cosh(J_{ij})$ for $i \neq j$, and $(C^{-1})_{ii} = 1 + \sum_{j \in \partial i} \sinh^2(J_{ij})$ (see [23] for the discussion on symmetry breaking in Cayley trees in the thermodynamic limit). This result can

be understood as a geometrical relation, where the connected correlation has a simple interpretation: for any two nodes i and j in a tree there is a unique path P_{ij} connecting them, and the correlation function can be written as $C_{ij} = \prod_{L_k \in P_{ij}} \tanh(J_{L_k})$ for $i \neq j$, and $C_{ii} = 1$, where L_k denotes links in this path. Note that in the expression for C_{ij} , if one replaces the multiplication by summation over the links, the correlation matrix then becomes the distance matrix in the weighted tree with weight $W_{ij} = \tanh(J_{ij})$. A similar expression for the inverse of the distance matrix is already well known in graph theory [24]. Bethe reconstruction then turns out to be particularly simple:

$$J_{ij} = -\frac{1}{2} \operatorname{arcsinh}[2(C^{-1})_{ij}], \quad (i \neq j). \quad (13)$$

It is clear from the above description that the computational expense of Bethe reconstruction is mostly due to the inversion of the correlation matrix, as is the case for MF, TAP and SM approaches. These methods are low computational expense methods, which are convenient to apply to systems of large sizes. The expense of inversion of the correlation matrix is of the order of N^3 for methods such as Gaussian elimination. On the other hand, the computation in a single update of SusP is already of the order of N^3 , which makes SusP slower due to the multiple iterative steps.

In the remainder of this note, we discuss the performance of Bethe reconstruction compared to MF, TAP, SM and SusP approaches, which we refer to as the mean-field family. Although IP is faster than those methods, it usually leads to estimates of couplings inferior to those from all of these methods, so no comparison with IP is made.

We will first compare the performance of these methods for a tree and for the Sherrington–Kirkpatrick (SK) model [25] in the absence of sampling noise (effectively an infinite number of patterns). Then the effect of sampling noise is considered for a particular case of sparse random graphs. The comparisons proceed as follows. We first construct a graph of N nodes, on which spins are located. Random values of couplings J_{ij}^0 are assigned to each edge, and random local fields h_i^0 are assigned at each spin. Two distributions for the random variables, the normal distribution with zero mean and standard deviation σ ($\mathcal{N}(0, \sigma^2)$) and the uniform distribution on the interval $[a, b]$ ($\mathcal{U}(a, b)$), will be used (see the corresponding figure captions). The magnetizations m_i^D and connected correlations C_{ij}^D are calculated either by enumerating all the spin configurations (infinite sampling) or by performing Monte Carlo simulation of the model at inverse temperature β to generate a finite number of M samples (finite sampling). The observed magnetizations and the connected correlations then serve as inputs for estimating the model parameters βh_i and βJ_{ij} (where we explicitly reintroduced the inverse temperature). Concentrating on the reconstruction of the couplings, we measure the deviation of each solution from the underlying couplings by means of the relative deviation

$$d(J_{ij}, J_{ij}^0) = \left[\frac{\sum_{i < j} (J_{ij} - J_{ij}^0)^2}{\sum_{i < j} (J_{ij}^0)^2} \right]^{1/2}. \quad (14)$$

Figure 1(a) shows the reconstructions of the Ising model on a Cayley tree of connectivity $z = 3$ with $N = 22$ spins. Here, the quality of Bethe reconstruction is limited only by the precision of numerical computations, confirming its exactness on a tree if the magnetizations m_i^D and the connected correlations C_{ij}^D are known exactly. SusP is also exact in this case, but fails at low temperatures [12]. On the other hand MF, TAP, and SM are all approximate, as seen particularly when the couplings are strong.

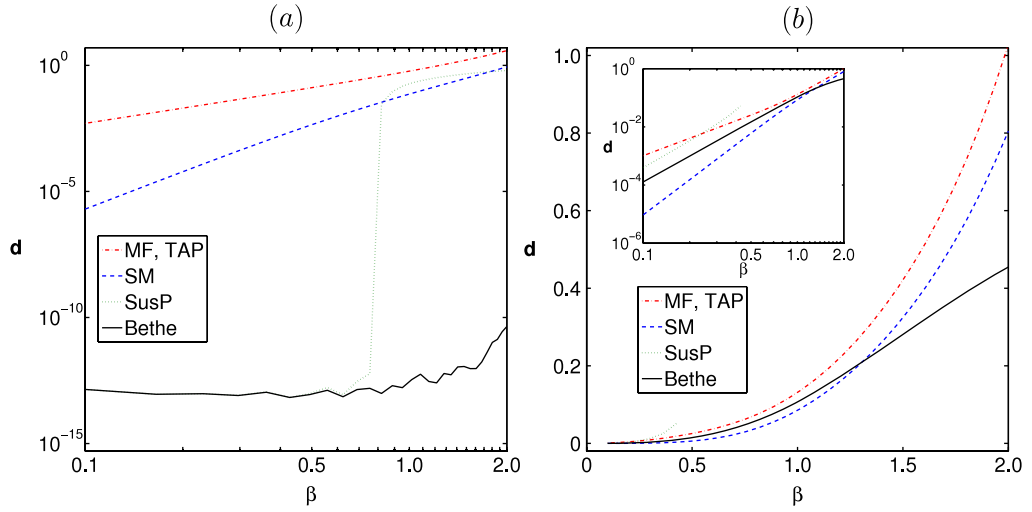


Figure 1. Benchmarking in the infinite sampling limit. Performance of the naive mean-field (MF), TAP (the same as the MF method in these cases), Sessak–Monasson (SM), susceptibility propagation (SusP) and Bethe reconstruction (Bethe) method, measured by means of the relative deviation d (see the main text) between the reconstructed couplings and the underlying couplings. (a) Cayley tree of connectivity $z = 3$ over $N = 22$ spins, $J_{ij}^0 \sim \mathcal{U}(-1, +1)$, $h_i^0 = 0$. (b) SK model of $N = 20$ spins, $J_{ij}^0 \sim \mathcal{N}(0, 1/N)$, $h_i^0 = 0$.

In figure 1(b) we turn to loopy graphs, and consider a particularly extreme case: the fully connected SK model of $N = 20$ spins. At weak couplings (small β), the differences between the reconstructions of all the methods and the underlying couplings are small, and in practice the differences between the methods will be obscured by sampling noise (see below). On the other hand, at strong couplings (larger β), Bethe reconstruction clearly outperforms all the other methods of the mean-field family. Interestingly, even inside the glassy regime, a finite overlap between the Bethe-reconstructed couplings and the underlying couplings persists. Note that SusP also follows the line of Bethe reconstruction closely at weak couplings, but at strong couplings it fails to converge to the Bethe solution.

We now consider the Ising model with $N = 50$ spins placed on the vertices of a random graph with fixed connectivity $z = 3$ [26]. Such graphs typically contain loops of length $\ln(N)$ [27, 28], but retain a locally tree-like structure. Figure 2(a) shows the results for a finite number of $M = 5000$ samples, where we omit SusP from the comparison due to its numerical instability. At weak couplings (corresponding to high temperatures), reconstruction by any method is limited by sampling noise. Remarkably, the sampling noise tends to smear out the small difference between SM and Bethe reconstructions for the entire weak coupling regime. Again, the deviation d of Bethe reconstruction increases only slowly through the strong coupling region, making it the best candidate for large couplings. Figure 2(b) probes the performances of the different methods at $\beta = 1.5$ with varying number of samples. The results show that all the reconstruction methods from the mean-field family are sensitive to the sampling noise. For the present system, it requires more than 700 samples to obtain a good reconstruction and to see a clear difference between the different methods.

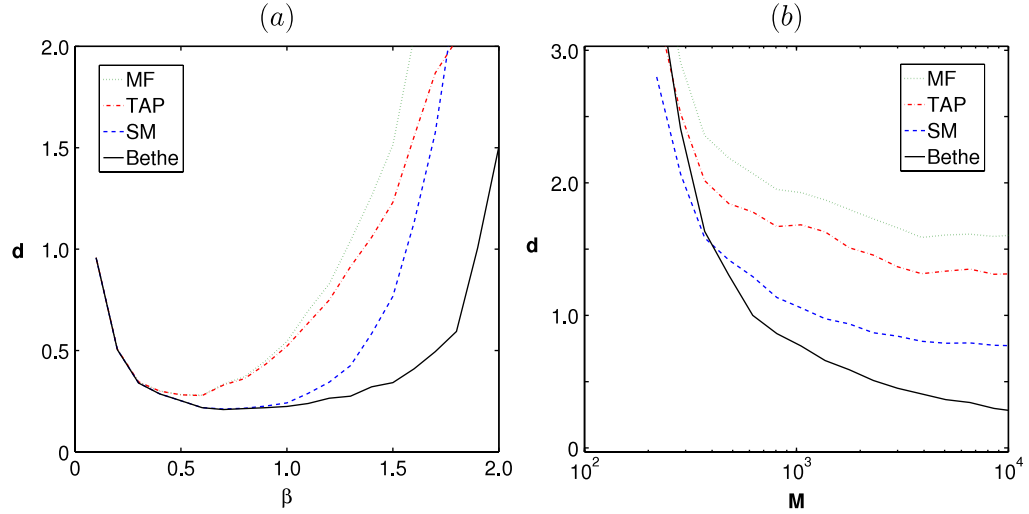


Figure 2. Benchmarking in the case of finite sampling. Performance of the naive mean-field (MF), TAP, Sessak–Monasson (SM) and Bethe reconstruction (Bethe) methods on a random graph with fixed connectivity $z = 3$, $N = 50$ spins, $J_{ij}^0 \sim \mathcal{U}(-1, +1)$, $h_i^0 \sim \mathcal{U}(-0.1, +0.1)$. (a) The deviation d versus the inverse temperature β , with $M = 5000$ samples. (b) The deviation d versus the number of samples M at $\beta = 1.5$.

In conclusion, we showed that the Bethe–Peierls approximation and linear response can serve as the basis for a method of the mean-field family for solving the inverse Ising problem. This Bethe reconstruction is not only computationally efficient but also stable through a wide range of couplings. While MF and TAP can be considered as expansions of low order in the couplings of Bethe reconstruction, the Sessak–Monasson reconstruction can be recovered by treating the parametric correlations in a particular manner. Although our observations suggest that susceptibility propagation and Bethe reconstruction are closely related, further work is needed to probe their relationship, in particular in the regime of strong couplings.

Since the Bethe–Peierls approximation works well for locally tree-like graphs, the extension of Bethe reconstruction to short-loop graphs, possibly resulting from the linear response applied to the Kikuchi approximation [17, 19, 29], is an interesting direction for future research. Another direction is extending the method to non-binary degrees of freedom, for which the linear response relation has been already studied [11].

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