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LETTER TO THE EDITOR

Intensively connected spin glasses: towards a replica-symmetry-breaking solution of the ground state

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Abstract. We propose a one-step replica-symmetry-breaking solution for spin glasses with finite connectivity. The introduction of two effective field distributions, one for each level of hierarchy, greatly simplifies the problem of manipulating an infinite set of order parameters. We then demonstrate the existence of a replica-symmetry-breaking solution more optimal than the replica-symmetric one and in better agreement with simulation results.

There has been recent interest in the study of spin glasses and the equivalent graph partitioning problem [1] in dilute spin systems, in which every site is bonded to a finite number of other sites [2-5]. In these studies, as for systems with *extensive* connectivities (i.e. the number of connected sites scales as N per site), the replica method [6] has become the standard technique, and within the replica-symmetric (RS) ansatz, the energy (or the cost function for the graph partitioning problem) is determined by the distribution of an auxiliary field, which corresponds to the effective field due to descendants in the Bethe approximation [7]. Such solutions give close but slightly lower ground-state energies when compared with simulation results [8].

Both theoretical and simulational arguments [9-13], however, have been proposed that the RS ground-state solution is unstable, just as in the case for the extensively connected SK model [14]. In the latter case, Parisi has shown that the true optimal solution can be approximated by a sequence of so-called replica-symmetry-breaking (RSB) solutions [15]. At each step of the solution, the order parameters $q^{\alpha\beta}$, representing the magnetisation overlaps between replicas α and β , are classified according to a hierarchical relation among the replicas, usually referred to as an ultrametric structure [16]. When the number of hierarchies increases to infinity, the solution is expected to be exact. Such sequences of solutions yield ground-state energies successively closer to simulation results. In the case of dilute spin systems, however, no such solutions have yet been proposed.

The major difficulty in finding the RSB ground state solution in dilute spin systems is that an infinite set of mean-field order parameters $\{q^{\alpha_1\alpha_2\cdots}\}$ is present. In the RS case, this set of infinite order parameters is expressed in terms of the moments of an auxiliary field distribution, and the manipulation is much simplified [3-5]. When the replica symmetry is broken, the number of distinct order parameters increases further and it remains unclear whether similar tricks can be applied.

Though little is known about the full RSB solution, it is illuminating to consider, as Parisi [17] did for the extensively-connected SK model, a one-step RSB solution. The purpose of this letter is to propose and demonstrate the existence of such a solution.

In the one-step RSB solution, the n replicas are ultrametrically related in two hierarchies. Replicas are divided into n/m subgroups, each of size m . Those belonging

to the same subgroup have stronger overlap, while those belonging to different subgroups have weaker overlap. As we shall see, this ansatz leads to ground-state energies higher than the RS solution, and subsequently closer to simulation results.

Let us formulate the problem specifically. Consider the Hamiltonian for a spin glass for N Ising spins,

$$\mathcal{H} = - \sum_{(ij)} J_{ij} S_i S_j \quad (1)$$

in which S_i ($1 \leq i \leq N$) takes the value ± 1 , and (ij) represents a pair of randomly chosen connected sites. The coupling strength J_{ij} follows a quenched distribution given by

$$f(J_{ij}) = \frac{1}{2} \delta(J_{ij} - J) + \frac{1}{2} \delta(J_{ij} + J). \quad (2)$$

For the case of fixed finite connectivity, in which every site is connected to precisely c other sites (c independent of N), we have derived an expression for the average free energy f using the replica method [5]†,

$$\beta f = \lim_{n \rightarrow 0} \frac{1}{n} \max \left[\frac{c}{2} \left(t_0 q_0^2 + t_1 \sum_{\alpha} q_{\alpha}^2 + t_2 \sum_{\alpha < \beta} q_{\alpha\beta}^2 + \dots - 1 \right) - \ln \text{Tr} \left(t_0 q_0 + t_1 \sum_{\alpha} q_{\alpha} S^{\alpha} + t_2 \sum_{\alpha < \beta} q_{\alpha\beta} S^{\alpha} S^{\beta} + \dots \right)^c \right] \quad (3)$$

where

$$t_r = \int dJ_{ij} f(J_{ij}) \cosh^n \beta J_{ij} \tanh^n \beta J_{ij} \quad (4)$$

and β is the inverse temperature, $\beta = (k_B T)^{-1}$.

To simplify the manipulation, we would like to express the infinite order parameters in terms of some field distribution. We therefore define a joint field distribution $P\{h^{\alpha}\}$ related to the order parameters via

$$q_{\alpha_1 \dots \alpha_r} = \left(\prod_{\alpha=1}^n \int dh^{\alpha} \right) P\{h^{\alpha}\} \tanh \beta h^{\alpha_1} \dots \tanh \beta h^{\alpha_r}. \quad (5)$$

The free energy can then be written as

$$\beta f = \lim_{n \rightarrow 0} \frac{1}{n} \max \left\{ \frac{c}{2} \int dJ f(J) \left(\prod_{\alpha} \int dh_1^{\alpha} dh_2^{\alpha} \right) P\{h_1^{\alpha}\} P\{h_2^{\alpha}\} \times \left(\cosh^n \beta J \prod_{\alpha} (1 + \tanh \beta J \tanh \beta h_1^{\alpha} \tanh \beta h_2^{\alpha}) - 1 \right) - \ln \text{Tr} \left[\int dJ f(J) \left(\prod_{\alpha} \int dh^{\alpha} \right) P\{h^{\alpha}\} \cosh^n \beta J \times \prod_{\alpha} (1 + \tanh \beta J \tanh \beta h^{\alpha} S^{\alpha}) \right]^c \right\}. \quad (6)$$

† We note that in the replica method for the extensively connected SK model, the maximum, rather than the minimum of the free-energy functional is sought, reflecting the fact that the number of $q^{\alpha\beta}$ parameters, $n(n-1)/2$, becomes negative in the limit as $n \rightarrow 0$. In the case of dilute spin systems, the situation is obscured by the presence of odd order parameters, namely q^{α} , $q^{\alpha\beta}$, etc, whose number is positive in the limit $n \rightarrow 0$. Here we restrict our discussion to the symmetric bond distribution prescribed by (2), in which the odd order parameters vanish. In this case, we still look for the maximum of the free-energy functional.

The previous RS solution [5] is equivalent to the ansatz

$$P\{h^\alpha\} = \int dh P(h) \prod_\alpha \delta(h^\alpha - h). \tag{7}$$

In the case of one-step RSB solution, it is instructive to quote well known results in the SK model, where we can write [17]

$$\langle s^{\alpha_1} \dots s^{\alpha_r} \rangle = \left(\prod_{\alpha=1}^n \int dh^\alpha \right) P\{h^\alpha\} \tanh \beta h^{\alpha_1} \dots \tanh \beta h^{\alpha_r}. \tag{8a}$$

where

$$P\{h^\alpha\} = \int \frac{dz}{\sqrt{2\pi pJ^2}} \exp\left(-\frac{z^2}{2pJ^2}\right) \times \prod_{j=1}^{n/m} \left\{ \int \frac{dy^{(j)}}{\sqrt{2\pi tJ^2}} \exp\left(\frac{(y^{(j)} - z)^2}{2tJ^2}\right) (2 \cosh \beta y^{(j)})^m \prod_{\alpha=(j-1)m+1}^{\alpha m} \delta(h^\alpha - y^{(j)}) \right. \\ \left. \times \left[\int \frac{dy^{(j)}}{\sqrt{2\pi tJ^2}} \exp\left(-\frac{(y^{(j)} - z)^2}{2tJ^2}\right) (2 \cosh \beta y^{(j)})^m \right]^{-1} \right\}. \tag{8b}$$

p, t, m are varied to optimise. Here we see immediately that the effective fields for the replicas obey an ultrametric relation. In other words, $h^\alpha = h^\beta$ only if α and β belong to the same subgroup of size m (i.e. $I(\alpha/m) = I(\beta/m)$ where $I(x)$ denotes the integer part of x). Each replica field is the sum of two terms, the field z , which is common to all replicas and obeys a Gaussian distribution of width \sqrt{pJ} , and the field $y^{(j)} - z$ ($j = 1 \dots n/m$), which is common to replicas belonging to the subgroup only, and obeys a Gaussian distribution of width \sqrt{tJ} .

For the dilute spin systems, it is therefore natural to expect an expression for $P\{h^\alpha\}$ similar to (8b), but with the Gaussian distributions replaced by some general field distribution, to be determined by the optimisation procedure in (6). Thus we write

$$P\{h^\alpha\} = \int dz \mathbb{P}(z) \left(\int dy \mathbb{T}(z, y) \prod_{\alpha=1}^m \delta(h^\alpha - y) \right) \dots \tag{9}$$

Putting $\mathbb{T}(z, y) = \delta(y - z)$ recovers the replica-symmetric solution.

Below, we consider a particularly simple form of (9), namely, that obtained by taking $\mathbb{P}(z)$ in (9) to be $\delta(z)$. This amounts to neglecting the correlation between various subgroups, and focusing our attention on the correlation within each subgroup. This reduces the free-energy expression to

$$\beta f = \max \left[-\frac{c}{2} \int dJ f(J) \ln \cosh \beta J + \frac{c}{2} \int dJ f(J) \frac{1}{m} \ln \int dy_1 \mathbb{T}(y_1) dy_2 \mathbb{T}(y_2) \right. \\ \times (1 + \tanh \beta J \tanh \beta y_1 \tanh \beta y_2)^m \\ \left. - \left(\prod_{s=1}^c \int dJ_s f(J_s) \right) \frac{1}{m} \ln \left(\prod_{s=1}^c \int dy_s \mathbb{T}(y_s) \right) \right. \\ \left. \times \left(\prod_{s=1}^c (1 + \tanh \beta J_s \tanh \beta y_s) + \prod_{s=1}^c (1 - \tanh \beta J_s \tanh \beta y_s) \right)^m \right]. \tag{10}$$

In view of the symmetric bond distribution (2), it is reasonable to restrict our attention to even distributions of $\mathbb{T}(y)$, which further reduce the free-energy expression to

$$\beta f = \max \left[-\frac{c}{2} \ln \cosh \beta J + \frac{c}{2m} \ln \int dy_1 \mathbb{T}(y_1) dy_2 \mathbb{T}(y_2) \right. \\ \left. \times (1 + \tanh \beta J \tanh \beta y_1 \tanh \beta y_2)^m - \frac{1}{m} \ln \left(\prod_{s=1}^c \int dy_s \mathbb{T}(y_s) \right) \right. \\ \left. \times \left(\prod_{s=1}^c (1 + \tanh \beta J \tanh \beta y_s) + \prod_{s=1}^c (1 - \tanh \beta J \tanh \beta y_s) \right)^m \right]. \quad (11)$$

Optimising this expression with respect to $\mathbb{T}(y)$ and m yields two self-consistency equations

$$\mathbb{T}(y) = \left(\prod_{s=1}^k \int dy_s \mathbb{T}(y_s) \operatorname{sech}^m \beta \xi_s \right) \left(2 \cosh \beta \sum_{s=1}^k \xi_s \right)^m \delta \left(y - \sum_{s=1}^k \xi_s \right) \\ \times \left[\left(\prod_{s=1}^k \int dy_s \mathbb{T}(y_s) \operatorname{sech}^m \beta \xi_s \right) \left(2 \cosh \beta \sum_{s=1}^k \xi_s \right)^m \right]^{-1} \quad (12a)$$

$$\frac{c}{2} \left(\frac{\int dy_1 \mathbb{T}(y_1) dy_2 \mathbb{T}(y_2) (1 + \tanh \beta J \tanh \beta y_1 \tanh \beta y_2)^m \ln(1 + \tanh \beta J \tanh \beta y_1 \tanh \beta y_2)^m}{\int dy_1 \mathbb{T}(y_1) dy_2 \mathbb{T}(y_2) (1 + \tanh \beta J \tanh \beta y_1 \tanh \beta y_2)^m} \right. \\ \left. - \ln \int dy_1 \mathbb{T}(y_1) dy_2 \mathbb{T}(y_2) (1 + \tanh \beta J \tanh \beta y_1 \tanh \beta y_2)^m \right) \\ = \left\{ \left(\prod_{s=1}^c \int dy_s \mathbb{T}(y_s) \right) \left[\left(\prod_{s=1}^c \operatorname{sech} \beta \xi_s \right) 2 \cosh \beta \sum_{s=1}^c \xi_s \right]^m \right. \\ \left. \times \ln \left[\left(\prod_{s=1}^c \operatorname{sech} \beta \xi_s \right) 2 \cosh \beta \sum_{s=1}^c \xi_s \right]^m \right\} \\ \times \left\{ \left(\prod_{s=1}^c \int dy_s \mathbb{T}(y_s) \right) \left[\left(\prod_{s=1}^c \operatorname{sech} \beta \xi_s \right) 2 \cosh \beta \sum_{s=1}^c \xi_s \right]^m \right\}^{-1} \\ - \ln \left(\prod_{s=1}^c \int dy_s \mathbb{T}(y_s) \right) \left[\left(\prod_{s=1}^c \operatorname{sech} \beta \xi_s \right) 2 \cosh \beta \sum_{s=1}^c \xi_s \right]^m \quad (12b)$$

where $k = c - 1$ and

$$\xi = \frac{1}{\beta} \tanh^{-1}(\tanh \beta J \tanh \beta y) \quad (13)$$

is the effective field at a site due to a field at one of its decedents.

It is more convenient to consider the field distribution $\mathbb{T}'(\xi)$ which is related to $\mathbb{T}(y)$ by

$$\mathbb{T}'(\xi) d\xi = \mathbb{T}(y) dy. \quad (14)$$

The ground-state energy is obtained as $T \rightarrow 0$. In this limit, the following form of m is appropriate:

$$m \xrightarrow{T \rightarrow 0} \gamma \frac{T}{J} \quad (15)$$

where γ is to be fitted optimally.

We note in passing that the m in the extensively connected case have the same form as $T \rightarrow 0$ [15].

The self-consistency equations (12a, b) then become

$$\begin{aligned} \mathbb{T}'(\xi) = & \left(\prod_{s=1}^k \int d\xi_s \mathbb{T}'(\xi_s) \right) \exp \left[-\frac{\gamma}{J} \left(\sum_s |\xi_s| - \left| \sum_s \xi_s \right| \right) \right] \\ & \times \delta \left[\xi - \text{sgn} \sum_s \xi_s \min \left(J, \left| \sum_s \xi_s \right| \right) \right] \\ & \times \left\{ \left(\prod_{s=1}^k \int d\xi_s \mathbb{T}'(\xi_s) \exp \left[-\frac{\gamma}{J} \left(\sum_s |\xi_s| - \left| \sum_s \xi_s \right| \right) \right] \right) \right\}^{-1} \end{aligned} \quad (16a)$$

$$\begin{aligned} & \frac{c}{2} \left(\frac{\int d\xi_1 \mathbb{T}'(\xi_1) d\xi_2 \mathbb{T}'(\xi_2) \exp[-\gamma(\sum_s |\xi_s| - |\sum_s \xi_s|)/J][\gamma(\sum_s |\xi_s| - |\sum_s \xi_s|)/J]}{\int d\xi_1 \mathbb{T}'(\xi_1) d\xi_2 \mathbb{T}'(\xi_2) \exp[-\gamma(\sum_s |\xi_s| - |\sum_s \xi_s|)/J]} \right. \\ & \left. + \ln \int d\xi_1 \mathbb{T}'(\xi_1) d\xi_2 \mathbb{T}'(\xi_2) \exp[-\gamma(\sum_s |\xi_s| - |\sum_s \xi_s|)/J] \right) \\ & = \frac{(\prod_{s=1}^c \int d\xi_s \mathbb{T}'(\xi_s)) \exp[-\gamma(\sum_s |\xi_s| - |\sum_s \xi_s|)/J][\gamma(\sum_s |\xi_s| - |\sum_s \xi_s|)/J]}{(\prod_{s=1}^c \int d\xi_s \mathbb{T}'(\xi_s)) \exp[-\gamma(\sum_s |\xi_s| - |\sum_s \xi_s|)/J]} \\ & + \ln(\prod_{s=1}^c \int d\xi_s \mathbb{T}'(\xi_s)) \exp[-\gamma(\sum_s |\xi_s| - |\sum_s \xi_s|)/J] \end{aligned} \quad (16b)$$

and the ground-state energy is given

$$\begin{aligned} -\frac{f}{J} = & \frac{c}{2} - \frac{c}{2\gamma} \ln \int d\xi_1 \mathbb{T}'(\xi_1) d\xi_2 \mathbb{T}'(\xi_2) \exp \left[-\frac{\gamma}{J} \left(\sum_s |\xi_s| - \left| \sum_s \xi_s \right| \right) \right] \\ & + \frac{1}{\gamma} \ln \left(\prod_{s=1}^c \int d\xi_s \mathbb{T}'(\xi_s) \right) \exp \left[-\frac{\gamma}{J} \left(\sum_s |\xi_s| - \left| \sum_s \xi_s \right| \right) \right]. \end{aligned} \quad (17)$$

We solve the self-consistency equations (16a, b) by a technique introduced previously [7], namely by allowing ξ to take integral multiple values of J/M (M integral) and letting $M \rightarrow \infty$. Thus

$$\mathbb{T}'(\xi) = T_0 \delta(\xi) + \sum_{i=1}^M T_i \left[\delta \left(\xi - \frac{i}{M} J \right) + \delta \left(\xi + \frac{i}{M} J \right) \right]. \quad (18)$$

Figure 1 shows the distribution function $\mathbb{T}'(\xi)$ for a trivalent spin glass. As in the RS case [7], it consists of delta function peaks at $\xi=0$ and $\pm J$ and a continuous component. Unlike the RS case, this continuous component has a downward kink at $\xi=0$. However, it is interesting to note that if we define an alternative distribution function $U(\xi)$ by

$$U(\xi) = \frac{\mathbb{T}'(\xi) \text{sech}^m \beta \xi}{\int d\xi \mathbb{T}'(\xi) \text{sech}^m \beta \xi} \quad (19a)$$

or inversely,

$$\mathbb{T}'(\xi) = \frac{U(\xi)(2 \cosh \beta \xi)^m}{\int d\xi U(\xi)(2 \cosh \beta \xi)^m} \quad (19b)$$

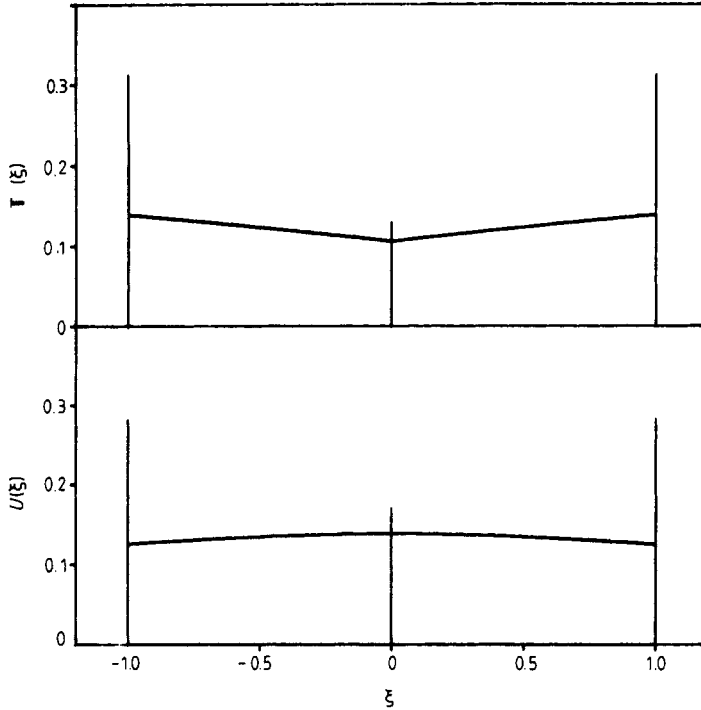


Figure 1. The functions $T(\xi)$ and $U(\xi)$ for a trivalent spin glass.

then $U(\xi)$ looks very similar to the distribution function in the RS case. Furthermore, substituting $U(\xi)$ into (9) shows that it plays the same role as the subgroup distribution of width $\sqrt{t}J$ in the extensively connected SK model (see (8b)). The significance of $U(\xi)$ is left for further study.

Table 1 shows the ground-state energy for $c = 3$ and 4. The one-step RSB solutions are higher than the corresponding RS ones. Hitherto, there has not been a direct study of the stability of the RS solution against replica-symmetry breaking. But since, in the replica method, we are looking for maxima of the free-energy expression, the existence of a more optimal RSB solution shows that the RS one is at best metastable and, most likely, unstable. Furthermore, the RSB solution gives a better agreement with simulation results (assuming the simulation results of the graph partitioning problem applies to the spin glass on the corresponding network).

In our one-step RSB solution, we have neglected the correlation between different subgroups by putting $\mathcal{P}(z)$ in (9) to be $\delta(z)$. Since, furthermore $T(\xi)$ is even, it is

Table 1. The ground-state energies for the trivalent and tetravalent spin glass. E_{RS} is the replica-symmetric solution obtained in [7]; E_{RSB} is given by (17); E_{SIM} is the simulation result in [8] obtained for the equivalent graph partitioning problem. The value of γ in (15) is also listed.

c	γ	$-E_{RS}/NJ$	$-E_{RSB}/NJ$	$-E_{sim}/NJ$
3	0.3720	1.2749	1.2720	1.260
4	0.3749	1.4833	1.4728	1.464

easy to see that the order parameters $q^{\alpha_1 \dots \alpha_r}$ are non-zero only if the number of replicas $\alpha_1 \dots \alpha_r$, within all the subgroups are even. It is interesting to compare this with a recent analysis of the p -spin model ($p \rightarrow \infty$) [13]. There, too, order parameters for subgroups containing odd numbers of replicas become zero in the zero-field limit.

Our solution, assuming uncorrelated subgroups, does not preclude the existence of other more optimal solutions, even within the one-step RSB ansatz. Such solutions will involve two distribution functions, $P(z)$ and $T(z, y)$, and self-consistency equations are not as easily separable as in (12a). Their existence is a subject for further study.

Although our analysis is done on systems with fixed finite connectivity, we expect the same replica-symmetry-breaking effect in systems with averaged connectivity, as long as the connectivity is sufficiently large. Our analysis also has implications to the graph bipartitioning problem. In this problem, we have a set of randomly connected sites, and the objective is to partition them into two subsets of equal size, so that the number of connections between the two sets (or cost function) is minimised. It has been shown [1, 4, 5, 18] that the problem is equivalent to finding the ground state of an Ising ferromagnet having the same connections but with a zero magnetisation. Assuming an even distribution of the effective fields, we expect the minimal cost function to correspond to the above spin glass solution. Recently, however, it was suggested [19] that the minimal cost function corresponds to an uneven field distribution instead. Nevertheless, we expect that such a solution can also be improved by the same replica-symmetry-breaking ansatz, and is undoubtedly a subject of future interest.

In summary, we have proposed a replica-symmetry-breaking solution for spin glasses with finite connectivity. In this ansatz, replicas are classified according to a hierarchy of subgroups. By associating an effective field with each subgroup of each level, the apparently intractable order parameters are expressed in terms of effective field distributions. In the particularly simple uncorrelated-subgroup ansatz, we find a solution more optimal than the RS solution. It is hoped that such a solution is a first step towards the full replica-symmetry-breaking solution.

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