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OVERLAP DISTRIBUTIONS AND TAXONOMY ANALYSIS OF SPIN GLASS STATES
WITH EQUAL WEIGHTS

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ABSTRACT

Techniques of numerical taxonomy are used to make ultrametricity tests of zero temperature states of the Sherrington-Kirkpatrick (SK) model. The states are considered with equal weights. Approximate trees are constructed by single- and complete-linkage procedures, and ultrametricity is measured by the difference of the corresponding distributions of the number of states in a cluster. The results are confronted with those of a model which is approximately ultrametric by construction. Other properties of the SK model with equal weights are also studied. In particular, the distribution of overlaps $P_J(q)$ and the distribution of $Y_J(q) = \int_q^1 P_J(q') dq'$ are evaluated. Fluctuations from sample to sample disappear.

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1. - INTRODUCTION

The nature of the spin glass transition of the Sherrington-Kirkpatrick (SK) model and its connection with the many-valley picture of the low-temperature phase have by now been clarified. As was shown recently, the order parameter is related to the probability distribution of the overlaps of those states¹⁾.

This interpretation led to further work where several interesting properties of the space of states were found²⁾. An important one is that it possesses an ultrametric topology, which implies the existence of a hierarchical tree associated to the states. Also relevant is the fact that the order parameter is not self-averaging, i.e., that it depends on the particular realization of spin couplings even in the infinite system limit. Numerical studies in this direction have also been carried out³⁾.

This progress in the understanding of the SK model properties has in turn motivated applications to other fields. In particular, the ultrametricity property could be important for optimization problems such as the "travelling salesman" problem or for models of associative memories [for a review of recent developments, see Ref. 4)].

Concepts and techniques developed for the SK model were used for the travelling salesman problem by Kirkpatrick and Toulouse⁵⁾. Giving a proper definition of the overlap between tours, they were able to compute various distributions of overlaps. However, an important difference between the two systems is the absence of Boltzmann weights in the travelling salesman problem. A more correct comparison with the SK model would require an analysis of the different overlap distributions of this model calculated with states weighed evenly.

Ultrametricity properties have also been incorporated in neural networks. The original models⁶⁾ choose the set of memories to be stored in the network as uncorrelated, i.e., approximately orthogonal when its number is small. However, the system should be able to store and recognize memories which have a finite overlap between them. A convenient way to achieve this is to organize the patterns in a hierarchical structure. Work in this direction was done very recently⁷⁾; memories were generated by a simple stochastic branching process which guarantees an approximate ultrametricity of the space of states, and they were learned by a modified Hebb's rule. Again, in this case the Boltzmann weights may not be adequate; patterns are recovered according to their attraction basin and this is the natural weight which should be given to them.

For these reasons it is necessary to understand the properties of the space of states of the SK model independently of the usual Boltzmann weights. Since these select the lowest energy states, a natural extension is to consider the set of the first N_S states with equal weight $1/N_S$. This is a difficult problem because analytical techniques cannot be applied, and in a numerical approach the lowest states are difficult to obtain for systems with more than $N \approx 30$ spins. The assignment of weights according to the attraction basin of the state is easier from the numerical point of view, and some of its properties have been studied⁸⁾.

In this paper we shall study properties of the zero temperature states of the SK model when they are given equal weights. We shall choose them as the N_S states of lowest energy found after applying a simple steepest-descent algorithm. Part of the work is dedicated to the analysis of ultrametricity: the construction of approximate hierarchical trees and the development of techniques to measure it. The SK model is compared with a system where ultrametricity is known to hold. Apart from this, we shall also evaluate the order parameter $P(q)$ and its fluctuations.

To analyze the possible existence of ultrametricity, we utilize techniques of numerical taxonomy^{9),4)} and employ them to determine hierarchical trees associated with the set of states. If ultrametricity holds only approximately, the distance between clusters of states is not well defined, and different criteria yield different trees. By adopting two extreme definitions, an idea of the degree of ultrametricity will be given by the similarity between the resulting hierarchies.

Once the trees are found, it is necessary to quantify their differences. We do this by evaluating the probability distribution f_q of the number of states in a cluster when the tree is cut at a given scale. This distribution, when considered at all scales, describes the whole tree. The final step is to perform the test for systems of different sizes and observe the behaviour of the difference $f_q^>(N) - f_q^<(N)$ of the distributions calculated with the two extreme realizations of the tree.

The numerical study has the inconvenience that it is very hard to find the states of lowest energies, and in fact we shall limit the analysis to 32 and 64 sites only. For this reason, and in order to support our conclusions, we shall apply the same technique to a more tractable model which is approximately ultra-

metric by construction⁷⁾. In this model, states are generated by a stochastic branching process which treats sites independently; this makes an analytical treatment possible, and it is easy to determine how it behaves as the number of states and the size of the system are changed. Although we consider only regular trees, more general ones can be analyzed immediately. This study will also lead us to detect possible sources of errors in the classification of states.

In the next section, after a brief description of a stochastic process which generates approximate ultrametric states, we solve it for the distribution of one and three overlaps. Sources of errors in the classification of states are also discussed.

Section 3 is devoted to the direct evaluation of $P(q)$ and ultrametricity tests of zero temperature metastable states of the SK model, taken with equal weights. Fluctuations of $P(q)$ are also calculated. Apart from their own interest, these results can be confronted with the same quantities evaluated through the tree structure.

Section 4 contains the description and application of the single and complete linkage techniques. Here we compare the results obtained for the simple model of Section 2 with those of the SK model. For both of them we evaluate the first moments of the distribution of states in a cluster. In particular for the second moment [which gives the probability that two states have an overlap larger than $q^{2)}$] we can make a comparison with the direct calculation, carried out in Section 3. Section 5 contains the conclusions.

2. - ANALYSIS OF A SIMPLE MODEL

Spin glass models are not easy to study numerically because of the difficulties of finding the states of lowest energy. For this reason it is convenient to have simple models for which ultrametricity is guaranteed by mechanisms similar to those appearing in the SK model. Here we discuss a model which will turn out to be tractable both numerically and analytically. It is inspired by recent work on the microstructure of the equilibrium states of the SK model¹⁰⁾ and was proposed and used to produce ultrametric neural networks⁷⁾.

After a brief discussion of its main features, we show how to solve it for the probabilities of one and three overlaps (although the technique can be used to obtain other distributions). This will allow us to extract conclusions about

the behaviour of ultrametricity as the number of states N_s or the size of the system N are changed.

Let us consider a system characterized by

- a) a tree, defined by a set of parameters such as the number of nodes and the number of branchings at each of them.
- b) N variables $\sigma_j = \pm 1$ defined on N sites. A state is specified by giving specific values to each of them, $s \equiv (\sigma_1, \sigma_2, \dots, \sigma_N)$.
- c) a stochastic process establishing a correspondence between a set of N_s states and the end of the branches, and such that it guarantees approximately the hierarchy dictated by the tree.

This system will have two kinds of parameters: those defining the geometry of the tree and those associated to the stochastic process itself. The dependence of the distributions on these parameters will turn out to be simple; as we shall see, the first ones will appear mainly as combinatorial factors, while the others can be absorbed into the probability P_i that, as a result of the process, a given site variable takes the value $+1$.

For clarity we shall limit the work to regular trees such that the nodes are distributed at B different levels, and at each of these all the branches split into the same number of new ones. We shall denote this number by b_k , where $k = 1, 2, \dots, B$ indicates the level. An example of this kind of tree is given in Fig. 1, where $B = 3$, $b_1 = 3$, $b_2 = 2$ and $b_3 = 3$.

As we mentioned before, the states are associated with the ends of the branches. By the nearest common ancestor of a set of states, we understand the nearest branch where all of them converge in the tree.

For purposes which will become clear soon, it is convenient to define the following sets of states:

- 1) the sets $\mathcal{C}_k$ ($k = 1, \dots, B$) contain all the pairs of states such that the ancestor of any of them is at level k ;
- 2) the sets $\mathcal{C}_{ijk}$ ($i, j, k = 1, \dots, B$) contain all triplets of states such that their three possible pairs are in $\mathcal{C}_i$, $\mathcal{C}_j$ and $\mathcal{C}_k$ respectively.

The fraction of pairs in $\mathcal{C}_k$ and of triplets in $\mathcal{C}_{ijk}$ are obtained after a

simple combinatorial analysis based on the tree structure. For instance, for $B = 3$ and a regular tree, the fractions of pairs are

$$\begin{aligned} c_1 &= \frac{(b_1 - 1) b_2 b_3}{N_s - 1} \\ c_2 &= \frac{(b_2 - 1) b_3}{N_s - 1} \\ c_3 &= \frac{b_3 - 1}{N_s - 1} \end{aligned} \quad (2.1)$$

with $N_s = b_1 b_2 b_3$. Of course, $\sum c_k = 1$. As N_s increases, these numbers converge to finite limits; in particular for $b_1 \rightarrow \infty$ all of them are zero except c_1 , which is one. The same is true for the fraction of triplets in the sets $\mathcal{C}_{ijk}$; in the same limit, only c_{111} is non-zero.

A measure of the similarity of two states is given by their overlap

$$q^{\alpha\beta} = 1/N \sum_{i=1}^N \sigma_i^{(\alpha)} \sigma_i^{(\beta)} \quad (2.2)$$

The height of the tree will be normalized to the maximum overlap ($q_M = 1$) and the position of its nodes at the k^{th} level will be defined as the mean value of the overlaps in $\mathcal{C}_k$.

We shall consider a stochastic process which does not correlate the sites, so then we can concentrate on only one of them. As a result of the process, we should obtain $\sigma_j^{(\alpha)}$ for all the states ($\alpha = 1, \dots, N_s$) and j fixed.

The generation of states starts at the base of the tree. In order to guarantee the hierarchical structure given by the tree, the process has to be identical for any pair of states until their nearest common ancestor is reached. After that it should proceed differently for each of them. The farther the ancestor is from the base, the smaller the differences between them are.

At the first level we define a probability distribution characterized by a mean value $\bar{y}_0 = h$ (which can be thought of as a magnetic field) and a variance

σ_0 . After drawing b_1 numbers $y_1^{(k)}$ ($k = 1, \dots, b_1$), the parameters $y_1^{-(k)}, \sigma_1$ of the distribution to be used at a given node of the second level are obtained as a function of the corresponding $y_1^{(k)}$. The procedure follows in this way until the last level is reached; the spin variables at the site j are determined as

$$\sigma_j^{(\alpha)} = \text{sign } y_B^{(\alpha)} \quad \alpha = 1, \dots, N_s \quad (2.3)$$

In this way, states with the nearest common ancestor at the last level are determined by the same distribution with parameters $y_{B-1}^{-(k)}, \sigma_{B-1}$ and their overlap is large. If the ancestor were at the previous level, the last distribution in common would be the one with mean $y_{B-2}^{-(k)}$ and from this point on, the states are determined differently. Finally, states with the common ancestors at the first level are obtained from distributions having only h in common, i.e., their only similarity is the overall magnetization.

We can now proceed to the evaluation of $P(q)$ and $P(q_1, q_2, q_3)$. Since the $\mathcal{C}_k$ are disjoint sets containing all the pairs, $P(q)$ can be split into B contributions

$$P(q) = \sum_{k=1}^B c_k P_k(q) \quad (2.4)$$

with $P_k(q)$ the probability that two states in $\mathcal{C}_k$ have overlap q .

Each of the $P_k(q)$ is a binomial distribution. Since sites are not correlated, the quantity

$$N_q = \sum_{i=1}^N \sigma_i^{(\alpha)} \sigma_i^{(\beta)} \quad (2.5)$$

can be thought of as the final position of a one-dimensional random walk. This is defined by a parameter p given by the probability that the spin variables $\sigma_1^{(\alpha)}$ and $\sigma_1^{(\beta)}$ have the same value. This is easily expressed in terms of the probability $P_{\uparrow}(\bar{y}_0, \bar{y}_1, \dots, \bar{y}_{B-1})$ that $\sigma_j^{(\gamma)} = +1$.

Notice that the division of pairs into the B classes $\mathcal{C}_k$ is appropriate for these considerations: all the overlaps of the pairs in $\mathcal{C}_k$ follow the same binomial distribution with a parameter p_k .

The probability that for n out of the N sites $\sigma_i^{(\alpha)} \sigma_i^{(\beta)} = +1$ is

$$P_k(n) = \frac{N!}{(N-n)! n!} p_k^{n-m} (1-p_k)^{N-n} \quad (2.6)$$

from which, using the relation between n and q , $Nq = 2n - N$, one immediately obtains $P_k(q)$. Its mean and variance are given by

$$\bar{q}_k = \langle q \rangle = 2p_k - 1 \quad (2.7)$$

$$\begin{aligned} \sigma_k^2 &= 4p_k(1-p_k)/N \\ &= \frac{1 - \bar{q}_k^2}{N} \end{aligned} \quad (2.8)$$

Since the interval between two consecutive values of q is $2/N$ while the dispersion is $O(1/\sqrt{N})$, $P_k(q)$ can be approximated by

$$P_k(q) dq = \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left[-(q - \bar{q}_k)^2 / 2\sigma_k^2\right] \quad (2.9)$$

σ_k gives us a measure of the indeterminacy of the position of the nodes at the level k . There is, however, another source of error in the model; since the distribution $P_k(q)$ will in general overlap, any attempt to classify pairs of states in the classes $\mathcal{C}_k$ will not be precise.

The distribution of three overlaps $P(q_1, q_2, q_3)$ can be treated in a similar fashion. In this case, we have to follow the evolution of the three overlaps simultaneously. For this purpose, it is convenient to classify the 2^3 possible values of the set $[\sigma_i^{(\alpha)}, \sigma_i^{(\beta)}, \sigma_i^{(\gamma)}]$ according to their net effect. In Fig. 2 we show the four possible cases explicitly; case a), for instance, corresponds to an increment of $+1$ in the three overlaps.

The probability associated with each case (p_a, p_b, p_c and p_d respectively) can again be determined as a function of the $P_{\uparrow}(\bar{y}_0, \bar{y}_1, \dots, \bar{y}_{B-1})$ and is the same for all triangles of states contained in a given class $\mathcal{C}_{ijk}$. This allows us to make the partition

$$P(q_1, q_2, q_3) = \sum_{i,j,k}^B \kappa_{ijk} P_{ijk}(q_1, q_2, q_3) \quad (2.10)$$

To simplify the notation we shall not attach the indices i, j, k to the p 's. The subsequent analysis is made for a fixed class $\mathcal{C}_{ijk}$.

As the process is repeated N times, each case will appear n_a, n_b, n_c and n_d times respectively; of course, these numbers satisfy

$$m_a + m_b + m_c + m_d = N \quad (2.11)$$

while for the p 's we have

$$p_a + p_b + p_c + p_d = 1 \quad (2.12)$$

It is clear that the n 's follow a multinomial distribution

$$P(m_a, m_b, m_c, m_d) = \frac{N!}{m_a! m_b! m_c! m_d!} p_a^{m_a} p_b^{m_b} p_c^{m_c} p_d^{m_d} \quad (2.13)$$

To obtain $P(q_1, q_2, q_3)$ we have first to relate these integers to q_1, q_2 and q_3

$$\begin{aligned} m_a &= N/4 (1 + q_1 + q_2 + q_3) \\ m_b &= N/4 (1 + q_1 - q_2 - q_3) \\ m_c &= N/4 (1 - q_1 + q_2 - q_3) \\ m_d &= N/4 (1 - q_1 - q_2 + q_3) \end{aligned} \quad (2.14)$$

Secondly, it is easy to realize that p_a, p_b, p_c and p_d can be expressed as functions of the B quantities p_k . Let us take as an example $B = 3$ and the set $\mathcal{C}_{322}$. We obtain

$$\begin{aligned} p_a &= (2p_2 + p_3 - 1)/2 \\ p_b &= p_c = (1 - p_3)/2 \\ p_d &= (-2p_2 + p_3 + 1)/2 \end{aligned} \quad (2.15)$$

and the final expression for P_{322} is

$$\begin{aligned} P_{322}(q_1, q_2, q_3) dq_1 dq_2 dq_3 &= \frac{dq_1 dq_2 dq_3}{(8\pi/N)^{3/2} (p_a p_b p_c p_d)^{1/2}} \cdot \\ &\cdot \exp \left\{ -N/8p_d (q_1 + q_2 - q_3 + 2p_3 - 4p_2 + 1)^2 - N/8p_a (q_1 + q_3 + q_2 - 4p_2 - 2p_3 + 3)^2 - \right. \\ &\quad \left. - N/8p_b (q_1 - q_2 - q_3 + 2p_3 - 1)^2 - N/8p_c (q_2 - q_1 - q_3 + 2p_3 - 1)^2 \right\} \end{aligned} \quad (2.16)$$

As $N \rightarrow \infty$, the distribution can again be given by Gaussians which approximate the following product of deltas:

$$P_{322}(q_1, q_2, q_3) \propto \delta(q_1 - q_2) \delta(q_2 - (2p_2 - 1)) \delta(q_3 - (2p_3 - 1)) \quad (2.17)$$

Remembering Eq. (7) for $\bar{q}_2$ and $\bar{q}_3$, this shows us how ultrametricity is recovered for all triangles in $\mathcal{C}_{322}$ as $N \rightarrow \infty$. The variance of each Gaussian is again of the form of Eq. (8).

As occurred for $P(q)$, the indeterminacy in the position of the nodes of the tree is not the only possible source of errors of the ultrametricity of this model. If the distributions $P_{ijk}(q_1, q_2, q_3)$ have a large overlap, errors in classifying all triangles of states will be large.

3. - THE SK MODEL WITH EQUAL WEIGHTS

Before presenting the taxonomy analysis of the model of the previous section and of the SK model, we make here a direct evaluation of $P(q)$ and of ultrametricity tests.

Apart from the main conclusion we obtain, i.e., that $P(q)$ does not fluctuate with our choice of weights, these results will be useful later for checking their agreement with the calculations based on the tree structure.

The technique is the same as in Ref. 3), the only difference being in the way the states are weighed. The Hamiltonian of the SK model is given by ($\sigma_i = \pm 1$)

$$H = \sum_{i>j}^N J_{ij} \sigma_i \sigma_j \quad (3.1)$$

and the couplings are random variables with a Gaussian distribution

$$P(J_{ij}) \propto \exp(-N/2 J_{ij}^2) \quad (3.2)$$

We concentrate on the zero temperature mean field equations

$$m_i = \text{sign} \left(\sum_j J_{ij} m_j \right) \quad (3.3)$$

from which m_i can take only the values ± 1 . Equation (3.3) is solved by a steepest-descent algorithm taking random starts. The N_s lowest-energy states found in this way are kept for the subsequent analysis.

All the solutions are given the same probability

$$P_\alpha = 1/N_s = z \quad (3.4)$$

with $\alpha = 1, \dots, N_s$, and the probability of one overlap is computed as

$$P_J(q) = z^2 \sum_{\alpha, \beta}^{N_s} \delta(q^{\alpha\beta} - q) \quad (3.5)$$

From it, we define the quantity

$$Y_J(q) = \int_q^1 P_J(q') dq' \quad (3.6)$$

and its average over all the samples

$$y(q) = \overline{Y_J(q)} \quad (3.7)$$

Finally, by a simple numerical analysis, one obtains the probability distribution $\pi_q(Y)$ of $Y_J(q)$.

In Figs. 3a and 3b, we show $P(q)$ for $N = 32$ and $N = 64$ for different values of N_s . Notice that, contrary to what happens when Boltzmann weights are included, the peak shifts to $q = 0$ as N_s is increased. This reflects the simple fact that the large number of solutions of Eq. (3.3) behave as uncorrelated spin configurations.

More important is the result for $\pi_q(Y)$. In Fig. 4, we can see that its maximum coincides with the average of $Y_J(q)$ over the samples. This is to be contrasted with the result of Ref. 2).

One can also do a simple test of ultrametricity. By explicit calculation, we first obtain the probability of three overlaps:

$$P_J(q_1, q_2, q_3) = 2^3 \sum_{\alpha, \beta, \gamma} \delta(q_1 - q^{\alpha\beta}) \delta(q_2 - q^{\alpha\gamma}) \delta(q_3 - q^{\beta\gamma}) \quad (3.8)$$

from where we evaluate the quantity³⁾

$$U = \frac{\int_0^{q_2} dq_1 \frac{P(q_1, q_2, q_3) (q_1 - q_2)^2}{\int_0^{q_2} dq_1 P(q_1, q_2, q_3)}}{\left(\frac{\int_0^{q_2} dq_1 (q_1 - q_2)^2}{\int_0^{q_2} dq_1} \right)^{-1}} \quad (3.9)$$

If there were no structure U would be 1, while for an ultrametric space it should approach 0.

The results for U are in Figs. 5a and 5b. What is surprising here is the small change of U under a variation by a factor 10 in N_s . This is in agreement with what was found in the previous section about the dependence on N_s of the distribution of overlaps; N_s and the tree structure entered mainly as combinatorial factors which eventually reach fixed values without affecting ultrametricity.

4. - CONSTRUCTION OF THE TREES

We now discuss a different way to study and quantify ultrametricity. For this purpose we shall introduce techniques which are usual in biological taxonomy⁹⁾; in particular we shall apply them to the states generated by the model described in Section 2 and to zero-temperature mean-field solutions of the SK model already used in Section 3.

When ultrametricity is not exact, one is faced with two main problems. First, it is not possible to assign unambiguously a tree to the set of states, and approximate ones have to be defined. Secondly, one has to find a way to measure the departure from ultrametricity. The first problem has been extensively studied, for instance to classify species with numerical taxonomy. Given a distance or similarity matrix between the objects to be classified, the technique consists of constructing two extreme trees such that they coincide with each other for ultrametric matrices. The differences between these two hierarchies give a measure of the degree of ultrametricity of the set of states.

At the smallest distance scale ($q = 1$), each state constitutes a cluster by itself, the distances between them being given by the similarity matrix. As the scale is increased, the first cluster to appear is the one formed by the two (or possible more) closest states. If ultrametricity were an exact property, any third state would form an isoscalar or equilateral triangle with those two. In this way, the distance between a state and a cluster (or more generally between clusters) is a well-defined concept.

When ultrametricity holds only approximately, there are two extreme ways to define those distances. They correspond to taking them systematically either as the smallest or as the largest one between the new state and those already in the cluster. These two cases are called single-linkage clustering and complete-linkage clustering respectively. For ultrametric systems, both procedures give the same tree.

Examples of trees resulting from the application of this technique to the SK model are shown in Fig. 6. They correspond to the five lowest energy states obtained for a given sample of spin couplings J_{ij} and $N = 32$. Notice that the two trees are qualitatively similar, the differences being essentially in the scales where new states are incorporated in a cluster. Divergences in the way a state is classified also appear, although they do not seem to occur frequently; this is, of course, a good sign for the existence of ultrametricity.

To determine to what extent the system departs from an ultrametric structure we need to define a way to measure the difference between the two procedures. To do this, we notice that a useful quantity to describe the tree structure is the cluster weight distribution, i.e., the probability $f(w, q)$ of having a cluster with weight w at a scale q . Such a quantity has been used to understand the properties of the SK model²⁾. The difference $f^<(w, q) - f^>(w, q)$ of the distributions obtained by the single- and complete-linkage procedures will give a measure of ultrametricity. [Although not applied to spin glass models, a different way to quantify ultrametricity was given by Rammal et al.¹¹⁾.]

The weight of the cluster I is defined as

$$w_I = \sum_{\alpha \in I} P_{\alpha} \quad (4.1)$$

where P_{α} is the weight of the state α . If the states have a uniform weight $z = 1/N_s$, this becomes proportional to the number of states n_I in the cluster I . By cutting the tree at different scales, it gives complete information about its structure.

The distribution of cluster weights $w_I = n_I z$ at the scale q is, for a given sample of spin couplings J^2 :

$$f_J(w, q) = \sum_I \delta(w - w_I) \quad (4.2)$$

and its moments in terms of n_I read

$$\begin{aligned} M_k(q) &= \int_0^1 w^k \overline{f_J(w, q)} dw \\ &= J^k \sum_I n_I^k \end{aligned} \quad (4.3)$$

and give the probability that k states are in the same cluster. In particular, $M_1 = 1$, and

$$M_2(q) = z^2 \sum_{\alpha, \beta} \overline{\theta(q^{\alpha\beta} - q)} \\ = y(q) \quad (4.4)$$

with $y(q)$ defined previously in Eq. (3.7). This is a quantity which is easily evaluated from the tree structure and it will allow us to make a comparison between the direct computation done in Section 3 and the technique described here.

We have first applied this procedure to the simple model of ultrametricity described in Section 2 to determine how it works and at which system size the single and complete linkage hierarchies converge to a common tree. For this model it is very easy to reach the value of N where this occurs; unfortunately, the same is not true for the SK model because the states with the largest attraction basin are not those with the lowest energies⁸⁾. As a consequence, we have restricted the application of the technique to rather small systems.

In order to generate approximately ultrametric states, we have to choose the distributions to be used at the B levels of the tree. As has already been explained, the parameters (mean and variance) of the distributions at the level k are determined as a function of the numbers drawn with the one at the previous level. As a simplifying assumption, we considered a finite number M of possible distributions at each level.

We studied a simple regular tree with $B = 2$, and took Gaussian distributions given by

$$P_h(y) \propto e^{-\frac{(y-h)^2}{2\sigma_0^2}} \\ P_{\bar{y}_{1,l}}(y) \propto e^{-\frac{(y-\bar{y}_{1,l})^2}{2\sigma_1^2}} \quad l=1, \dots, M \quad (4.5)$$

for the first and second levels respectively. We took $M = 4$, and the corresponding values $\bar{y}_{1,l}$ were determined from $P_h(y)$ by dividing the interval $(-\infty, \infty)$ into four pieces of equal probability $\mathcal{Q}_l$, then

$$\bar{y}_{1,2} = \int_{\mathcal{D}_2} dy \, y P_2(y) / \int_{\mathcal{D}_2} dy \, P_2(y) \quad (4.6)$$

The variances were fixed at $\sigma_0 = 0.5$ and $\sigma_1 = 0.25$. Finally, we took $h = 0$ and $N_s = 10$ with $b_1 = 2$ and $b_2 = 5$. For these values of the parameters, the average overlaps in the sets $\mathcal{C}_1$ and $\mathcal{C}_2$ are $\bar{q}_1 = 0$ and $\bar{q}_2 = 0.6$ respectively.

In Fig. 7, we show our result of the first moments M_k for this model. The tree was cut at $q = 0.5$. The data correspond to the single- and complete-linkage techniques for $N = 32$ and 64 . Notice that for these sizes the difference of the two procedures is still large, although it is smaller for 64 sites.

For this model, the numerical analysis can be carried out up to values of N for which the tree becomes well defined. Furthermore, the moments can be easily obtained as the probability that k states are in the same cluster; for $q < \bar{q}_2$ the result reads

$$M_k(q) = 1/2^{k-1} \quad (4.7)$$

Calling $M_k^<$ and $M_k^>$ the moments calculated with the single-linkage and the complete-linkage techniques respectively, for this model we can define the ratio

$$d_k(q) = (M_k^<(q) - M_k^>(q)) / 2^{k-1} \quad (4.8)$$

This is shown in Fig. 8 for different values of N up to $N = 300$.

From Fig. 7, we notice that the single-linkage results are closer to the exact values than the complete-linkage ones. Although not shown in this Figure, for $N = 300$ $M_k^<(0.5)$ turns out to be identical to the exact number.

In Fig. 9, we compare $y(q)$ (with $q = 0.5$) given by $M_2^<$ and $M_2^>$ with its direct calculation based on the evaluation of $P(q)$ as described in Section 3 for the SK model. The latter always remains between the single- and complete-linkage results. Again for $N = 32$ and 64 , the differences between these numbers are large, although they decrease with N .

In the next Figure (Fig. 10), we show the moments $M_k^<$ and $M_k^>$ for the SK model. Notice that these curves are qualitatively similar to those of Fig. 7. The single-linkage result is always larger than the complete-linkage one, and presents only small variations with N . The difference $M_k^< - M_k^>$ again decreases with N .

The second moment can again be compared with the value of $y(q)$ obtained by the direct evaluation of $P(q)$ made in Section 3 (see the Table). For $N = 32$, $y(q)$ is between $M_2^<$ and $M_2^>$, as before. For $N = 64$, it is slightly bigger than $M_2^<$; however, we have to remember that for 64 spins it is very unlikely that we are studying the lowest-energy states, which are probably further from the ground state than for $N = 32$.

For comparison purposes, we show in Fig. 11 the moments of the distribution obtained for the SK model with normal weights. This was found analytically by Mézard et al.²⁾, who obtained

$$\overline{f_y(w, y)} = \frac{\omega^{y-2} (1-\omega)^{-y}}{\Gamma(y) \Gamma(1-y)} \quad (4.9)$$

for the distribution and

$$M_k = \frac{\Gamma(k+y-1)}{\Gamma(y) \Gamma(k)} \quad (4.10)$$

for its moments. In the Figure, the second moment was chosen equal to our direct evaluation of $y(q)$ for $N = 32$ [$y(q) = 0.495$]. As k increases, these moments differ substantially from those of Fig. 10. The differences are also clear in the distribution of cluster weights. For the case of equal weights, the behaviour is as follows: at small q ($q \sim 0.1$) there are two clusters, resulting in a rather flat distribution, symmetric around $w = 0.5$ but increasing rapidly at the edges. As the scale is taken larger, the number of clusters increases very slowly (it is 2.06 at $q = 0.5$); the moments are practically unchanged and are given by those in Fig. 10. For larger q , the number of clusters changes more rapidly (for $q = 0.7$ there are about 3.5), and the distribution of cluster weights becomes a delta at the value N_s^{-1} .

5. - CONCLUSIONS

In this work we have discussed several properties of the SK model in the absence of Boltzmann weights. The order parameter $P(q)$ and the probability distribution of $Y_J(q)$ have been obtained by a direct evaluation. Ultrametricity was tested both directly and by use of the single- and complete-linkage procedures.

The behaviour of $P(q)$ and $\pi_q(Y)$ changes drastically when the states are assigned equal weights, indicating that the properties found in Ref. 2) are due to the Boltzmann weights. In particular, $\pi_q(Y)$ is peaked at the average value of Y , showing the disappearance of the fluctuations of $P_J(q)$ from sample to sample. The peak of $P(q)$ moves to $q = 0$ as more states are included, but this can be easily understood by the fact that the states behave as uncorrelated spin configurations.

A direct test of ultrametricity [U , as defined in Ref. 3)] gives, for a small number of states and $N = 32$, numbers compatible with those obtained with Boltzmann factors included. For a larger N this quantity decreases, but less than was found in Ref. 3). However, it is surprising that even large sets of states respond rather well to the test, giving a value of U which departs only slightly from the one of smaller sets. The analysis of a simple model agrees with this; for that model, ultrametricity becomes exact as $N \rightarrow \infty$, but is independent of N_s .

We have also performed a numerical taxonomy analysis of the states. Once approximate trees are constructed by means of the single- and complete-linkage procedures, quantities can be evaluated using the tree structure. The distribution of cluster weights obtained behaves, with the size of the system, like the model of ultrametricity. The analysis was, however, carried out for a rather small number of states ($N_s = 10$). This distribution is different from the case with Boltzmann factors. In particular for large scales ($q \sim 1$), the clusters are essentially the states and, while for the normal SK model one expects an exponential distribution of independent levels¹²⁾, for the present case it is simply $\delta(W - N_s^{-1})$.

Let us remark that this work was done looking only at the states of lowest energy we could find, although we weighed them evenly. Probably for states chosen differently the conclusions for $P(q)$ and $\pi_q(Y)$ will still hold, since they depend

crucially on the absence of Boltzmann weights. On the other hand, the result of the ultrametricity tests could change, since this property might depend more strongly on the detailed structure of the lowest-lying states.

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N	$\langle M_2$	$\rangle M_2$	$y(q)$
32	0.690	0.360	0.495
64	0.672	0.543	0.705

Table

The second moment of the distribution of the number of states in a cluster evaluated with the single- and complete-linkage procedures and $y(q)$ obtained as described in Section 3, for the SK model. The trees were cut at the scale $q = 0.5$.

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FIGURE CAPTIONS

- Fig. 1 : A regular tree, with $B = 3$, $b_1 = 3$, $b_2 = 2$, $b_3 = 3$.
- Fig. 2 : The eight possible configurations of three spins, classified according to their contribution to the three overlaps.
- Fig. 3a) : $P(q)$ for the SK model with equal weights for the N_s lowest states. The curves correspond to $N_s = 15$ ($\bullet$), $N_s = 30$ (+) and $N_s = 50$ (Δ), and $N = 32$ spins;
- 3b) : idem with $N_s = 30$ (+), $N_s = 150$ ($\bullet$) and $N_s = 300$ (x), for $N = 64$ spins.

- Fig. 4 : Probability distribution of Y for $q = 0.3125$ [$y(q) = 0.471$] and 32 spins. Notice that the maximum coincides with the average $y(q)$. Here $N_s = 30$ (+) and $N_s = 50$ (Δ).
- Fig. 5a) : The ultrametricity test U for $N = 32$. $N_s = 15$ (o), 40 (x) and 50 (Δ);
- 5b) : idem for $N = 64$. The number of states is $N_s = 30$ (+), $N_s = 150$ (o) and $N_s = 300$ (x).
- Fig. 6 : Examples of trees obtained with the single- and complete-linkage procedures. a) single-linkage, b) complete-linkage, $N_s = 5$ and $N = 32$.
- Fig. 7 : The moments of the distribution of the number of states in a cluster for the model of ultrametricity of Section 2, calculated with the single- and complete-linkage trees:
For $N = 32$: single linkage ($\cdot$), complete linkage (o)
For $N = 64$: single linkage (+), complete linkage (x)
(at the scale $q = 0.5$).
- Fig. 8 : The ratio $d_k = (M_k^{\langle} - M_k^{\rangle})/2^{k-1}$ as a function of N for $k = 2$ ($\cdot$), $k = 3$ (+), $k = 4$ (o) and $k = 5$ (x) (at the scale $q = 0.5$).
- Fig. 9 : Comparison of $M_2^{\langle}$ and $M_2^{\rangle}$ with $y(q)$ for $q = 0.5$ as a function of N (for the model of ultrametricity). $M_2^{\langle}$ ($\cdot$), $M_2^{\rangle}$ (o), direct calculation (x).
- Fig. 10 : The moments $M_k^{\langle}$ and $M_k^{\rangle}$ for the SK model.
For $N = 32$: single linkage ($\cdot$), complete linkage (o)
For $N = 64$: single linkage (+), complete linkage (x).
- Fig. 11 : The moments M_k for the SK model with normal weights according to Eq. (10); $y(q) = 0.495$.

$$b_1 = 3$$

$$b_2 = 2$$

$$b_3 = 3$$

Fig. 1

Fig. 2

Fig. 3a

Fig. 3b

Fig. 4

Fig. 5a

Fig. 5b

Fig. 6

Fig. 7

Fig. 8

Fig. 9

Fig. 10

Fig. 11