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Fractal geometry of spin-glass models

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Abstract

The topology of the phase space of spin glasses can be conveniently condensed into a tree structure, termed a barrier tree, whose tips are the local minima and whose internal nodes are the lowest-energy saddles connecting the local minima. For the mean-field Ising spin glass with p-spin interactions and sizes up to $N = 24$ spins we compute exactly the weight distribution $\psi(w)$, where $w = w(s)$ is the fraction of minima that are connected through the saddle s. For low-energy saddles we find a power law $\psi(w) \sim w^{-D}$, where D is the fractal dimension of the phase space, and barrier trees which are qualitatively similar to balanced random trees. For higher energy levels, on the other hand, the barrier trees become highly unbalanced resulting in a flat weight distribution.

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1. Introduction

Two key features that any successful model of biological evolution ought to possess are stability and diversity, i.e. exactly the properties responsible for the complex thermodynamics of spin glasses [1,2]. It is not a surprise therefore, that many of the tools and concepts of the statistical mechanics of disordered systems have been applied to the study of the evolutionary process. In this contribution we show that such interchange can be profitable to statistical mechanics too, in that a great deal of information about the phase space of spin-glass models can be condensed into a tree structure, in a standard procedure widely used in taxonomy and molecular phylogenetics [3]. As in the biological case, the statistical properties of this tree can be used to characterize the disordered system quantitatively.

The main unifying concept in the investigations of the physics of disordered systems and evolutionary change is probably the notion of a fitness or energy landscape. The concept of

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neighbourhood among genotypes (configurations), typically defined such that point mutations interconvert neighbours, allows us to view the set of all genotypes as the vertices of a graph with edges connecting neighbouring configurations. A *fitness landscape* is then obtained by assigning a fitness value to each vertex. An explicit connection between those two research fields is obtained in the case of populations of asexually reproducing haploid organisms evolving on rugged fitness landscapes. In this case the genotypes are often modelled by configurations of N Ising spins $s = (s_1, \ldots, s_N)$ with $s_i = \pm 1$ so that a point mutation corresponds to a single spin flip. In the simplest case, evolutionary adaptation is described as an 'adaptive walk' on the fitness landscape [4], whose statistical mechanics equivalent is the zero-temperature Glauber dynamics. The fitness function assigns a random numerical value to each one of the 2^N spin configurations. In this work we consider the p-spin landscapes [5]:

$$\mathcal{H}_p(s) = -\sum_{1 \leqslant i_1 \leqslant i_2 \cdots \leqslant i_N \leqslant N} J_{i_1 i_2 \ldots i_N} s_{i_1} s_{i_2} \ldots s_{i_N} \tag{1}$$

where the $J_{i_1 i_2 \ldots i_N}$ are statistically independent Gaussian distributed random variables with mean zero and variance $p\,!/(2N^{p-1})$. The p-spin models form a class of tunably rugged landscapes similar to Kauffman's Nk-model [4], which is not only more appealing to statistical mechanics but also is a more natural basis of landscape theory [6]. For $p = 2$ the Hamiltonian $\mathcal{H}_p$ reduces to the SK model [7] which exhibits a large number of highly correlated local minima, while the limit $p \to \infty$ corresponds to the random energy model (REM) [5] and yields an extremely rugged, uncorrelated landscape. Like the Nk-model, p-spin landscapes have been used repeatedly to model evolutionary processes (see, for example, [1, 8, 9]). For some recent work on the structure of the energy surface of p-spin models we refer to, for example, [10–13].

2. Basins and barriers

The nontrivial breaking of ergodicity in spin glass systems is usually described by the so-called many-valley scenario in which the ease with which one valley can be reached from another one depends on the saddle points connecting them. More specifically, the energy of the lowest saddle point separating two local minima x and y is

$$E[x, y] = \min_{\boldsymbol{p} \in \mathbb{P}_{xy}} \max_{z \in \boldsymbol{p}} \mathcal{H}_p(z) \tag{2}$$

where $\mathbb{P}_{xy}$ is the set of all paths $\boldsymbol{p}$ connecting x and y by a series of subsequent spin-flips. The saddle-point energy $E[\cdot, \cdot]$ is an ultrametric distance measure on the set of local minima (see , for example, [14]).

Let us assume for a moment that the energy function is non-degenerate, i.e. $\mathcal{H}_p(x) \neq \mathcal{H}_p(y)$ whenever $x \neq y$. This is true for generic p-spin models with odd interaction order p. Then there is a unique saddle point $s = s(x, y)$ connecting x and y characterized by $\mathcal{H}_p(s) = E[x, y]$. Note that this definition of saddle point is more restrictive than in differential geometry where saddles are not required to separate local optima [15]. To each saddle point s there is a unique collection of configurations $B(s)$ that can be reached from s by a path along which the energy never exceeds $\mathcal{H}_p(s)$. In other words, the configurations in $B(s)$ are mutually connected by paths that never go higher than $\mathcal{H}_p(s)$. This property warrants to call $B(s)$ the *valley or basin below the saddle* s. Furthermore, suppose that $\mathcal{H}_p(s) < \mathcal{H}_p(s')$. Then there are two possibilities: if $s \in B(s')$ then $B(s) \subseteq B(s')$, i.e. the basin of s is a 'sub-basin' of $B(s')$, or $s \notin B(s')$ in which case $B(s) \cap B(s') = \emptyset$, i.e. the valleys are disjoint. This property arranges the local minima and the saddle points in a unique hierarchical structure which is conveniently represented as a tree, termed *barrier tree* (see figure 1).

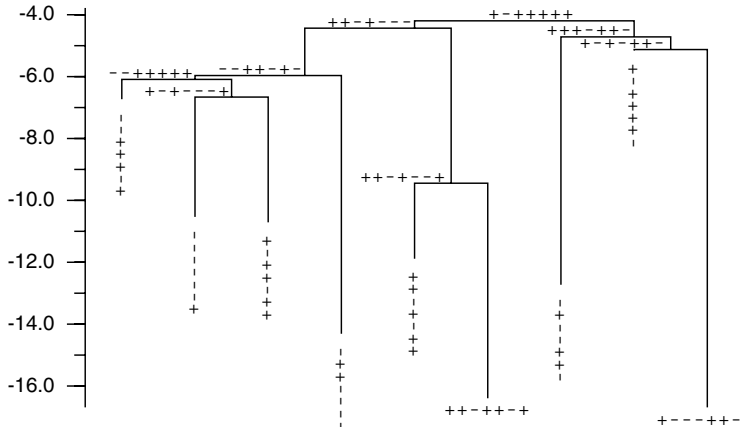

Figure 1. Barrier tree for a 3-spin model with $N = 7$. The nine minima (tips) and eight connecting saddle points (internal nodes) are labelled by their spin configurations.

In principle, barrier trees can be computed by means of the following simple recursive procedure: the tips of the tree are the local minima. The parent of tip x is the lowest-energy saddle point s that connects x to another local minimum. Analogously, the parent of a saddle point s is another saddle point s' that connects s to a local minimum z that is not contained in the basin below s, i.e. $z \notin B(s)$. The 'root' of the resulting tree is the saddle point s^* with the highest energy, since by definition all local minima are contained in $B(s^*)$. Note that the subtree $\mathfrak{T}(s)$ that has the saddle s as its root has exactly the local minima in $B(s)$ as its tips.

The exact calculation of the barrier tree for *discrete* systems is a highly challenging computational problem and only recently some progress in that direction has been achieved, mainly in the context of RNA and protein folding [16, 17]. The reason is that, unless one has sufficient *a priori* knowledge on the landscape, it is necessary to generate the complete landscape in order to find all local minima. Even for very small system sizes a simple-minded exhaustive search approach to evaluating equation (2) would be hopeless as one must calculate all paths connecting all pairs of minima. In fact, the exact evaluation of these paths was qualified as 'desperately hard' in a bold earlier study of the energy barriers of the SK model [18].

The program package `barriers-0.9` instead constructs the barrier tree directly from an energy sorted list of all spin configurations [16]. Starting with the lowest energy configurations, `barriers-0.9` explicitly builds the basins $B(s)$ and subtrees $\mathfrak{T}(s)$ by checking for each configuration whether it (a) is a local minimum, (b) uniquely belongs to the basin of a local minimum that was encountered earlier in the list, or (c) 'merges' two or more basins, i.e. whether it is a saddle point. We refer to [13] for a detailed account of the algorithm in the spin-glass context[5]. Since both CPU time and memory requirements increase only linearly with the number of configurations, our approach is at present feasible for landscapes with up to about 10^8 configurations, i.e. for Ising spin systems with up to about $N = 27$ spins. Our statistical investigations are limited to $N \leqslant 24$ to keep the CPU requirements reasonable. In contrast, methods for exploring the *continuous* energy surfaces of molecules and molecular clusters, for which exact enumeration is impossible, use incomplete databases of minima, transition states, and their connecting rearrangements. When searching transition states starting from a given minimum, these numerical techniques make explicit use of the fact that the potential energy

[5] The software is available from http://www.tbi.univie.ac.at/∼ivo/RNA/Barriers/

surface is a manifold (see e.g. [19–22]). Thus they are not applicable to the discrete setting considered here.

The definition of barrier trees becomes more complicated when the energy function is degenerate as in the case of p-spin models with even p, where $\mathcal{H}_p(s) = \mathcal{H}_p(-s)$. In this case we have to identify the saddle points s and s' with the same interior node of the tree provided: (i) they have the same energy and (ii) they are connected by a path along which the energy does not exceed $\mathcal{H}_p(s) = \mathcal{H}_p(s')$ [23]. In the non-degenerate case the trees are almost always binary, i.e. each internal node is connected to two nodes (saddle or minima) only in its valley. Degeneracies can occur also for geometric reasons since the same saddle point can connect more than two basins. One may, however, 'expand' a non-binary interior node into a sequence of binary nodes at the same height. We use this technical trick here to simplify the computations and, since our results are practically independent of the parity of p, it does not seem to produce any spurious effects.

3. Sub-tree weight distribution

One important and widely used aggregate characteristic of a tree is the weight distribution of its saddles or subtrees $\psi(w)$, where the weight $w = w(s)$ is, in the simplest case, just the fraction of minima or tips in $B(s)$. For instance, analysis of frequency distributions of taxonomic units containing various numbers of subunits (e.g., species per genus) were found to be well described by power laws [24], thus pointing out the fractal nature of those hierarchies.

It is instructive to first consider some examples of simple trees. One extreme case is the deterministic asymmetric binary tree of depth $m > 1$ in which every 'left' child is a tip. The tree has $2m - 1$ nodes: m tips and $m - 1$ saddles, and each weight between $2/m$ and 1 appears exactly once. Hence

$$\psi(w) = \frac{1}{m-1} \qquad \text{for} \quad 2/m \leqslant w \leqslant 1. \tag{3}$$

In the other extreme is the completely balanced deterministic binary tree of depth $m \geqslant 1$: it has $2^m - 1$ nodes, of which 2^{m-1} are tips and the remaining $2^{m-1} - 1$ are saddles. It can be easily shown that there are 2^{m-k-1} saddles with weights $w = 2^{k-m+1}$; $k = 1, \ldots, m-1$, so that

$$\psi(w) = \begin{cases} \dfrac{1}{w}\left(2^{1-m} - 1\right) & \text{if} \quad \log_2 w \in \mathbb{N} \\ 0 & \text{if} \quad \log_2 w \notin \mathbb{N}. \end{cases} \tag{4}$$

Another case of interest is the balanced random binary tree, which can be generated as follows: starting with m nodes (in the beginning all nodes are tips), pick two of them randomly, say x and y, and connect them by a saddle z; then replace x by z and remove y from the node list. This procedure is repeated until the node list contains only one element, which becomes the root. We find that a power law

$$\langle \psi(w) \rangle \sim w^{-D} \tag{5}$$

with $D \approx 2$ fits the average weight distribution extremely well almost in the entire range of $w \in (0, 1)$ (see figure 2, lower-right panel).

We turn now to the analysis of the complex trees associated with the random energy function (1) as produced by the program `barriers-0.9`. In this case the average number m of tips increases exponentially with the number of spins $\mathrm{e}^{\alpha_p N}$, where the 'complexity' α_p increases from $\alpha_2 = 0.199$ to $\alpha_\infty = \ln 2$ [2]. Log–log plots of the average weight distributions of subtrees for particular p-spin models and the REM are shown in figure 2. Except perhaps

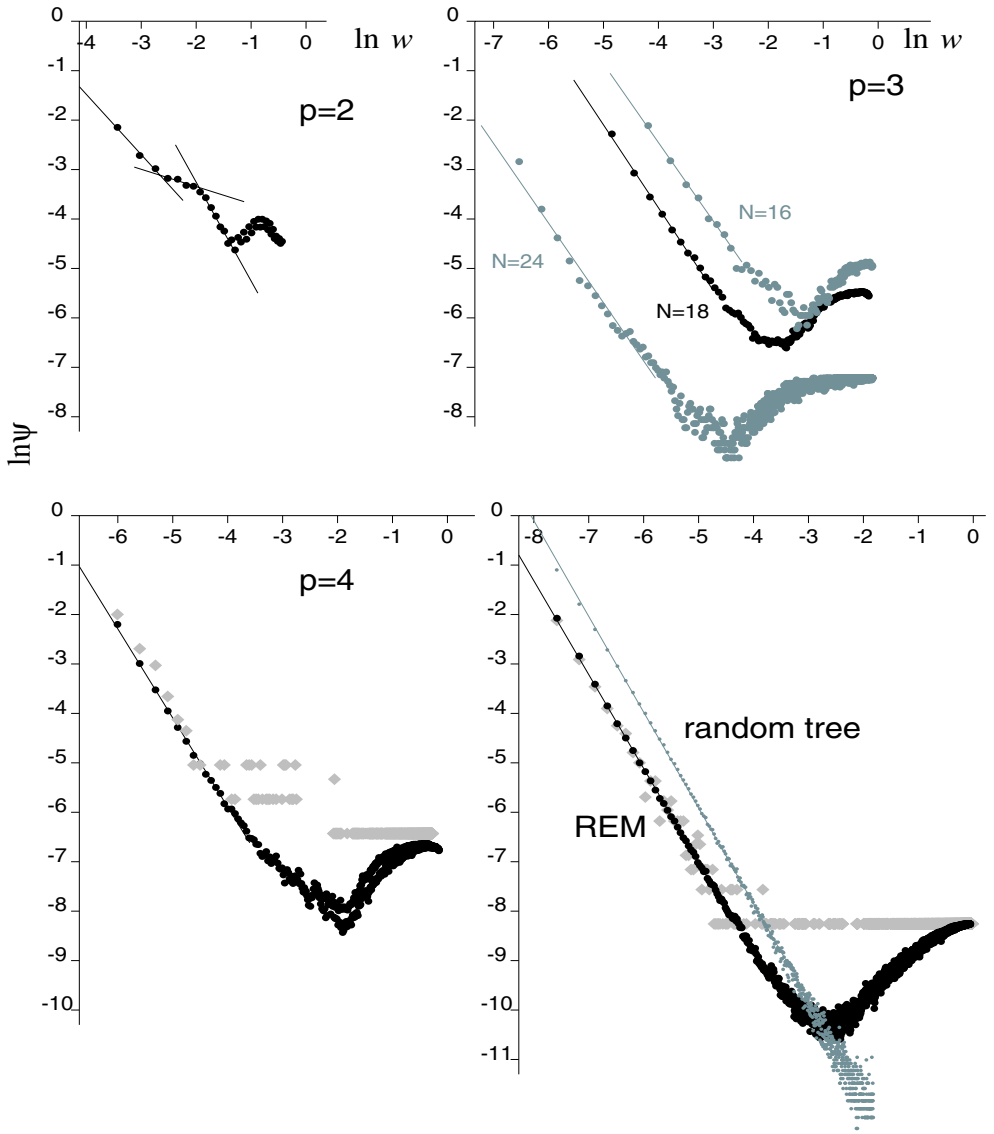

Figure 2. Log–log plots of the average frequency of subtrees with different fractions of tips for the p-spin landscapes with $N = 18$, and the REM with $N = 16$, averaged over 300 landscapes each. The distributions for a single landscape (grey diamonds) are also shown for $p = 4$ and the REM, while for $p = 3$ we show data for three different sizes N. The weight distribution for a random balanced tree with $m = 10\,000$ tips is shown for comparison.

for $p = 2$, the data are very well fitted by straight lines with negative slopes in the regime of high frequencies, suggesting then a power law form (5) with $D \approx 2$ (see figure 3). Here D can be viewed as the fractal dimension of the barrier tree and hence of the phase space of the disordered system. Thus there are many subtrees (saddles) with few tips (minima) and few subtrees with many tips. In other words, the trees are approximately balanced in this regime. To illustrate the effects of finite size, the panel for $p = 3$ shows data for three values of N, pointing out the robustness of the power-law behaviour to variation of system sizes. In addition,

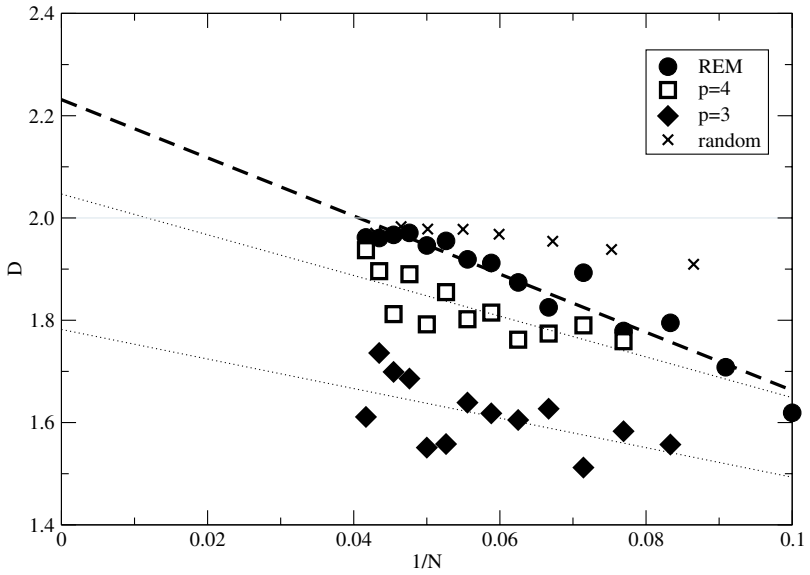

Figure 3. Dependence of the exponents D on the reciprocal of the number of spins N. The data for $p = 2$ do not allow for the unambiguous estimate of an exponent D. For the random trees we fix the horizontal axis by setting $N = \log_2 m$.

as illustrated by the grey data points in the panels for $p = 4$ and the REM, the same scaling law also seems to hold for the weight distribution of a single instance of the landscape.

The low-frequency regime, associated to high-energy saddles near the root of the tree and hence to weights close to 1, is also very interesting. In fact, the flat weight distribution $\psi(w) \sim 1/m$ observed in single-landscape statistics shows that the tree become extremely unbalanced near the root, thus indicating the existence of high-energy local minima which are directly connected to saddles that contain almost all tips of the tree. The minimum in $\langle\psi(w)\rangle$ comes from the fact that in the intermediate-frequency regime not all possible values of the weights are observed for a single landscape, while near the root we find almost all weights exactly once (see panel for $p = 4$ in figure 2) and so $\langle\psi(w)\rangle$ must increase with w for large weights. In the size-range of the landscape considered here the number of balanced (low-energy, high-frequency) saddles and of unbalanced (high-energy, low-frequency) saddles is comparable.

It is important to realize that even for the REM the barrier trees are not random balanced trees as one might expect. The main distinguishing feature is the transition from a balanced barrier tree close to the ground state to an unbalanced structure at high-energy levels. This transition occurs at lower levels of the tree in the more correlated spin glasses. We note that this finding is consistent with the observation that the basin sizes of the metastable states are correlated with their energies, even for the REM (see, for example, figure 5 in [13]). Moreover, it should be stressed that the scaling law (5) is by no means a mere consequence of the existence of an underlying tree structure. This is illustrated by the study of discrete branching processes which generate different forms of weight distributions [25], and by the asymmetric binary tree example discussed above.

The average weight distribution for the SK model displays a rather distinct behaviour pattern which seems to indicate the existence of two different types of self-similar structures at different levels of the tree. These results, however, must be taken with caution since the

weight statistics is greatly impaired by the fact that the trees are typically very small in this model. For instance, for $N = 18$ the average number of tips is about 50 in the SK model as compared to the $\sim 10^5$ tips in the REM.

An attempt to estimate D for infinite system sizes is presented in figure 3. From these data one cannot discard the possibility that for very large systems the exponents will converge to $D = 2$ independently of p. The estimate of D for larger systems must resort to a stochastic approach which focuses on the distribution of saddles connecting a set of sampled minima (see [15] for work in this line). The main shortcoming of applying that kind of approach to study weight distributions is that a reliable statistics requires a very large number of sampled minima (on the order of 10^5), turning then unviable the Monte Carlo approach used to obtain the paths of minimum energy cost connecting the minima [15, 18].

4. Concluding remarks

The replica theory predicts a similar hierarchical structure for the space of pure states, consisting of clusters within clusters. In particular, Parisi's prescription for the matrix of configurational overlaps between pure states q_{ab} yields the following probability density that a cluster has weight W (defined in terms of the free energy of the corresponding pure state) [2]

$$f(W) = \frac{W^{y-2}\,(1-W)^{-y}}{\Gamma(y)\Gamma(1-y)} \tag{6}$$

which for small weights reduces to a power law $f(W) \sim W^{y-2}$. Here $y \in (0, 1)$ is a complicated function of the physical parameters p and the temperature T. For instance, for the REM one has $y = 1 - T/T_c$, where $T_c = (4 \ln 2)^{-1/2}$. However, this description holds for nonzero temperatures only: at $T = 0$ the q_{ab} must become equal to 1 and all fine details of the cluster structure are lost. In contrast to the replica approach, our analysis of the phase space of spin glasses through their corresponding barrier trees is based on natural physical quantities—saddle points and minima—which are well defined at zero temperature.

The hierarchical organization of the saddle points which form an ultrametric space seems a natural realization of the well known scenario of glassy relaxation in which many relevant degrees of freedom relax hierarchically leading to a wide spectrum of characteristic times and hence to the typical slow relaxation observed in glassy materials [26]. Interestingly, the spectrum of relaxation times may be a fractal object as well, both because explicit models of diffusion by hopping in ultrametric space give rise to such hierarchical relaxation [27, 28], and because we expect that the fractal nature of the weight distribution of saddles carries over to the size distribution of barrier heights between minima. In this context we note that numerical simulation on moderate-size landscape show that transition rates between valleys can be estimated quite accurately from the barrier trees alone [29].

Regardless of the conjectured physical consequences of our findings, to the best of our knowledge, they provide the only direct evidence that the phase space of spin-glass models exhibits a fractal geometry at low-energy levels, where the barrier trees are essentially fully balanced random trees. In addition, the finding that for high-energy levels the barrier trees become completely unbalanced unveils an unexpected asymmetry between the energy valleys of the mean-field spin glasses.

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