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Multiscale analysis of hierarchical landscapes

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Abstract

The Statistical Mechanics calculation of the Gibbs–Boltzmann partition function does not give all the necessary information for a complete analysis of a rugged energy hypersurface. We show instead, that the partition function of a conveniently defined system composed of a number of replicas constrained to lie at specific distances provides such a description. We further sketch how the usual Replica formalism can be used to calculate these more complicated functions. As a by-product we show that in this way unstable solutions in the usual Replica method acquire a new meaning.

Keywords: Hierarchical landscapes; Multiscale analysis; Gibbs–Boltzmann partition function; Replica formalism; Rugged energy hypersurface; TAP solutions

1. Introduction

We want to analyze the general properties of a rugged energy hypersurface. In general it will consist of a valley structure whereby a certain number of valleys fall inside a larger valley. Let us then imagine a generic contour plot of such a surface (see Fig. 1). We could be interested in understanding how many E contour curves with entropy S lie inside an $E' > E$ closed curve of entropy S'. This information is relevant, for instance, for the relaxational dynamics of the system. However, this information cannot be derived from the usual partition function

$$Z_J = \sum_{\{C\}} e^{-\beta H_J[C]}, \tag{1}$$

where there is one single parameter (β). In fact, the Z function aggregates the information that we would like to keep apart. The subscript J reminds us that in the definition of H_J there are an infinite number of random parameters and that, therefore, we are trying to analyze statistically the properties of an ensemble of hypersurfaces. The results will take the form of analytic expressions for average quantities including correlations among local minima at variable distance in configuration space. From now on we will omit the J subscript. Average values over J are denoted by an upper bar.

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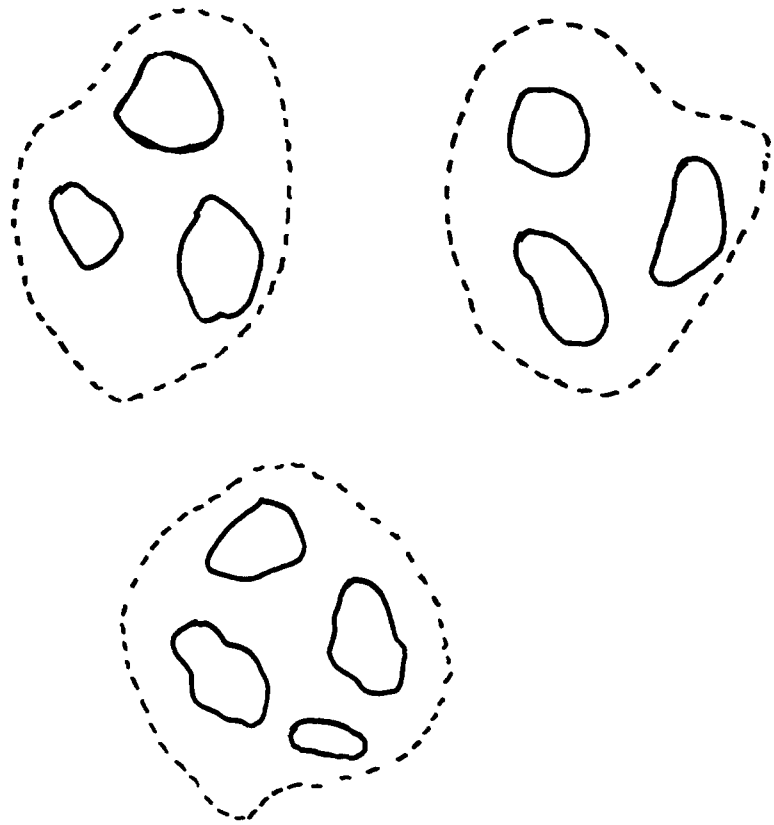

Fig. 1. The plane represents configuration space. Full closed lines delimit a valleys, dashed lines delimit supervalleys/clusters.

The temperature in Z selects a level energy. Furthermore, in the presence of valleys of different depths it also selects the free energy of the latter and therefore does not "see" smaller or shallower valleys because they do not have enough weight and larger or deeper ones because of their reduced number.

In Section 2 we will show how to introduce another parameter in the partition function that will allow us to consider separately the contributions coming from valleys with different free energies.

Still this additional parameter is not sufficient to answer questions involving simultaneously valleys at two different energies of the type discussed in the first paragraph. In Section 3 we will show how to generalize the prescription to include these more complicated cases.

In Section 4 we address the question of how to calculate these generalized Z functions. We show that it requires a subtle generalization of the Replica method that, however, leads to the same functional of the overlap matrix that appears in the usual Replica equations. The new parameters appear as constraints that keep the overlap matrix "off equilibrium".

2. Derivation of the number of valleys (TAP solutions) with a certain free energy

For this purpose we propose calculating the partition function of a system composed of R Replicas, all of which have mutual overlap q. That is

$$Z_R(\beta, q) = \sum_{\{C_1, C_2, \ldots, C_R\}} e^{-\beta \sum_{a=1}^{R} H[C_a]} \prod_{a,b} \delta(C_a C_b - q), \tag{2}$$

where $C_a C_b$ is the overlap between the configurations C_a and C_b. For the time being R is larger than 1 and integer. If q is chosen such that the R configurations fall into the same valley then

$$\log Z_R(\beta, q) = -\beta R E + R S_V + \log \mathcal{N}_V, \tag{3}$$

where E is the internal energy, S_V the valley entropy while $\mathcal{N}_V$ is the number of valleys.

From this formula it is obvious that we have thus succeeded in disagregating the total entropy into two components; the number of configurations per valley and the number of valleys. In addition the new partition function has three parameters: β, R, q. However, it should be obvious that fixing β and R one is fixing which configurations contribute in every valley. If we choose q different from the most probable value for such configurations, changing R will have a dramatic effect. In fact, in our calculation we observed that we could analytically continue Eq. (3) only if q was chosen to be the one that maximizes $Z_R(\beta, q)$ (although this could be a consequence of the simple choice of the ansatz for the Q matrix).

In any case, analytically, continuing (3) in R for $q = q_{EA}$ defined by

$$\frac{\partial \log Z_R(\beta, q_{EA})}{\partial q_{EA}} = 0 \tag{4}$$

one can derive

$$F_V = \frac{-1}{\beta} \frac{\partial \log Z_R}{\partial R}, \tag{5}$$

$$\mathcal{N}_V = \log Z_R + \beta F_V \tag{6}$$

and therefore by substitution, or more easily through a Legendre transformation, we derive the number of valleys as a function of their free energy.

Parenthetically we observe that the bottom of any valley is determined by the equation:

$$S_V(E_{\text{bottom}}) = 0. \tag{7}$$

It is then evident that F_V is the linear extrapolation estimate of E_{bottom} from an expansion of S_V around E.

We have calculated Z_R and analytically continued it for the p-spin spherical model and derived the well known formulas of Crisanti–Sommers [1]. In Section 4 we will sketch the derivation.

Here we want to stress again that Z_R probes configurations that never contribute to Z for any temperature. Thus we can study the lowest lying configurations of valleys that lie high in the energy hypersurface or vice versa.

3. Clusters of valleys or valleys inside valleys

To understand the dynamics one would like to know whether valleys tend to remain at a distance of each other or tend to appear in clusters. A related question concerns the number of valleys of a certain type inside a supervalley of a different type.

In this section we want to address both questions.

Towards that goal we now consider R' Replicas of R systems such that the latter are constrained to have an overlap q, while Replicas belonging to different groups have an overlap $q' < q$.

If we refer to Fig. 1 where the dashed closed curves represent a loosely defined supervalley limit or else the boundary of the cluster we immediately notice that now the number of valleys is decomposed in two components: number of valleys belonging to a supervalley ($\mathcal{N}_{\mathcal{V}\in\mathcal{V}'}$) and the number of supervalleys ($\mathcal{N}_{\mathcal{V}'}$).

Then

$$Z_{RR'}(\beta,q,q') = \sum_{\{C_{a,b};a=1\cdots R;b=1\cdots R'\}} \mathrm{e}^{-\sum_{a,b} H[C_{ab}]} \prod_{aa'b} \delta(C_{a,b}C_{a',b} - q) \prod_{aa'bb'} \delta(C_{ab}C_{a'b'} - q') \tag{8}$$

is decomposed into

$$\log Z_{RR'}(\beta,q,q') = -\beta RR'E + RR'S_{\mathrm{V}} + R'\log\mathcal{N}_{\mathcal{V}\in\mathcal{V}'} + \log\mathcal{N}_{\mathcal{V}'} \tag{9}$$

From this we can derive the equivalent of a free energy for the cluster/supervalley as a linear extrapolation for the free energy of the lowest lying valley in the cluster

$$S_{\mathcal{V}'/\mathcal{V}} = \log\mathcal{N}_{\mathcal{V}\in\mathcal{V}'} = 0. \tag{10}$$

In fact, replacing in (9) we obtain

$$\log Z_{RR'}(\beta,q,q') = -\beta RR'F_{\mathrm{V}} + R'\log\mathcal{N}_{\mathcal{V}\in\mathcal{V}'} + \log\mathcal{N}_{\mathcal{V}'} \tag{11}$$

from which we can derive

$$\frac{\partial\log\mathcal{N}_{\mathcal{V}\in\mathcal{V}'}}{\partial F_{\mathrm{V}}} = \beta R, \tag{12}$$

so that the free energy of the supervalley is

$$G_{\mathcal{V}'} = F_{\mathcal{V}} - (\beta R)^{-1}\log\mathcal{N}_{\mathcal{V}\in\mathcal{V}'}. \tag{13}$$

It is interesting to notice that configurations inside a valley are weighed by the Boltzmann–Gibbs parameter β, while valleys inside supervalleys use the parameter βR and supervalleys are weighed with $\beta RR'$. The variables E, $F_{\mathcal{V}}$, $G_{\mathcal{V}'}$ are related to β, βR, $\beta RR'$ through Legendre transformations.

4. Sketch of the $\overline{\log Z_R}$ calculation

We will here describe the calculation of $\overline{\log Z_R}$ from which one can obtain the average number of valleys as a function of their free energy. The calculations of $\overline{\log Z_{RR'}}$ is considerably more cumbersome but not more difficult.

We will show that the calculations needed for this approach are contained in the usual Parisi solution [2] though it requires the consideration of specific unstable solutions to the saddle point equations of the mean field approach.

For definiteness let us consider the following Hamiltonian:

$$H = -\sum_{i_1>i_2>\cdots>i_p} J_{i_1 i_2\cdots i_p} s_{i_1} s_{i_2}\ldots s_{i_p}, \tag{14}$$

where the s_i can be Ising variables or real variables subject to a spherical constraint.

Both Z and Z_R will depend on J and must be averaged over these variables. It is well known that one has to average the $\log Z_R$ and $\log Z$. To do that one begins calculating $\overline{Z^n}$ and $\overline{Z_R^n}$ and ends up continuing analytically n to zero. Thus for Z one has to replicate the system n times, while for Z_R one replicates $n \times R$ times. But

in both cases the functionals $A(Q)$ that appear after averaging over J and summing over the $\{S_{i_a}\}$ are formally identical

$$\overline{\log Z} = \text{saddle point } \{e^{NA(Q)}\},$$
$$\overline{\log Z_R} = \text{saddle point } \{e^{NA(Q_R)}\},$$

where Q is an $n \times n$ matrix with zero on the diagonal while Q_R is an $(n \times R) \times (n \times R)$ with zero on the diagonal and q_{EA} on the block $R \times R$ matrices along the diagonal. As n goes to zero and q_{EA} must be varied it turns out that the saddle point equations are identical. However, there are two subtle differences. First of all R corresponds here to an additional Parisi's m variable, however, it is not restricted to be less than one and most important it should not be varied. Second, when analyzing the stability one does not have to consider second order variations in q_{EA}. In fact, for $p \geq 3$ and for $T > T_c$ it turns out that in the $\overline{\log Z}$ calculation only the Replica symmetric solution is stable while for $\overline{\log Z_R}$ and $R > 1$ the solution with one Replica symmetry breaking becomes stable and gives the leading contribution.

A straightforward calculation for the p-spin spherical model gives the Crisanti–Sommers formula for the number of valleys as a function of free energy [2,3].

5. Conclusions

In a previous contribution one of us [4] has shown that an analysis of this type leads to a careful control of Simulated Annealing. But perhaps the most interesting consequence of this approach is the fact that it assigns a clear physical meaning to unstable solutions of the Replica method equations that pop out continuously in the literature. We are particularly interested in the one Replica symmetry breaking solution that plays a crucial role in the ageing dynamics of the p-spin spherical model [5]. We plan to go back to this problem.

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