On the replica symmetry for random weighted matchings

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Abstract. We present an extensive simulation on random weighted matchings dealing with the possible existence of the breaking of the replica symmetry. Using the so-called post-opimal analysis of combinatorial optimization we are able to draw the definite conclusion on the replica behaviour for this class of problems by computing the probability distribution of the overlaps $P(q)$ and through the careful check of our sampling of configuration space.

1. Introduction

In this paper we discuss the nature of the replica solution of random weighted matching problems [1, 2].

We know that the replica symmetry breaking solution for the Sherrington–Kirkpatrick model (see reprints in [2]) is a necessary step to discuss a physically sensible theory. The appearance of ultrametric organization of phase space is one of the main features of the replica symmetry-breaking pattern. Even if we do not yet know if this behaviour persists in real physical dimensions (although there are some numerical simulations whose conclusions seem in agreement with this view [7, 8]) its existence in infinite dimensions shows a remarkable difference between the 'classical' conceptions derived from usual homogeneous Ising-like models. The behaviour of the probability distribution $P(q)$ for the overlap, q, between different spin configurations at fixed temperature, is, for example, one of the main differences with which it is usually possible to determine a spin-glass behaviour.

It seems very natural, therefore, to discuss the properties of the random weighted matching models following the same pattern. We shall be concerned with, essentially, two main objects. First of all the aforementioned probability distribution of the overlap $P(q)$, then with the distribution of the difference between the energy of the ground state, which we know exactly for every sample, and the energies of the 'excited' states. To have a spin-glass behaviour we should find a $P(q)$ with a tail that extends down to $q = 0$ even at the thermodynamical limit. This paper, following our previous one [3], is its complement by addressing questions left aside in it.

2. Random matching problems

We start with a graph whose elements are primarily vertices and links connecting them. We shall be concerned with the problem of fully connected and unoriented graphs, which means that we have an unoriented link for every pair of vertices. If we put a weight to each link our goal is to match vertices only by pairs (it means that on each vertex must arrive one and only one link) but with the constraint that the total weight of the matching be the least possible (we restrict the discussion to the simple matching case, leaving the bipartite case as understood; see however [3]). It is possible to use concepts from statistical mechanics to deal with this problem [2]. We introduce an Ising-like variable n_{ij}, symmetric, and whose values label the presence, $n_{ij} = 1$, or the absence, $n_{ij} = 0$, of the link connecting vertex i to vertex j in the seeked matching (where $i, j = 1, \ldots, 2N$). If we denote by l_{ij} the weight of this link we can write the partition function as

$$Z = \sum_{\{n_{ij}\}} \prod_{i<j} (T_{ij})^{n_{ij}} \tag{1}$$

where

$$T_{ij} = \exp(-\tilde{\beta} l_{ij}) \tag{2}$$

is the Boltzmann weight, but with the configurations of the Ising-like variables subject to the constraint

$$\sum_{i=1}^{2N} n_{ij} = 1 \tag{3}$$

which tells us that only one link should leave from each vertex. It is obviously possible to generalize it by putting K, a positive integer, instead of 1, which means that from each vertex leave K links.

To deal with the random matching case we can take two roads: we distribute the vertices on a unit hypercube or the links with an 'opportune' distribution. In this paper we shall deal with the second case leaving the first (otherwise called Euclidean matching [4]) to a forthcoming publication.

The distribution should be taken with care because it should give us a sensible thermodynamic limit. This task has been recently discussed by Vannimenus and Mézard [5] who said that the correct probability distribution is governed by its behaviour near the $l = 0$ weight,

$$P(l) \approx l^r \tag{4}$$

and the right low 'temperature' behaviour, which prevents the entropy dominating the whole range of 'temperatures', is obtained with the rescaling

$$\tilde{\beta} = \beta N^{\delta} \tag{5}$$

where $\delta = 1/(r+1)$.

It is clear that we face the problem of how to calculate the thermodynamic functions, e.g. the free energy, free from sample fluctuations. The theory of disordered systems says that the right procedure is to average the free energy over the probability distribution for the weights, i.e.,

$$\beta \bar{F} = -\overline{\log Z} \tag{6}$$

where the overbar means just the average over the $\{l\}$.

The most important tool utilized in this context is the replica method. It consists in computing the above free energy by using the following trick,

$$\overline{\log Z} = \lim_{n \to 0} \frac{\overline{Z^n} - 1}{n} \tag{7}$$

where Z^n is nothing but the partition function of n non-interacting replicas of the initial system. Now, it is possible to calculate simply the free energy (see, e.g., [2]), and the conclusion is, for large N,

$$\overline{Z^n} = \int \prod_{p=1}^{n} \prod_{a_1 < \ldots < a_p} \frac{\mathrm{d}q_{a_1 \ldots a_p}}{\sqrt{2\pi N g_p}} \exp N \left[-\frac{1}{2} \sum_{p=1}^{n} \frac{1}{g_p} \sum_{a_1 < \ldots < a_p} (q_{a_1 \ldots a_p})^2 + 2 \log \mathscr{Z} \right] \tag{8}$$

where $g_p = (p\beta)^{-(r+1)}$ and $\mathscr{Z}$, the one-site partition function, is,

$$\mathscr{Z} = \int_0^{2\pi} \frac{\mathrm{d}\lambda_1}{2\pi} \cdots \int_0^{2\pi} \frac{\mathrm{d}\lambda_n}{2\pi} \exp \left[i \sum_{a=1}^{n} \lambda_a + \sum_{p=1}^{n} \sum_{a_1 < \ldots < a_p} q_{a_1 \ldots a_p} e^{-i(\lambda_{a_1} + \ldots + \lambda_{a_p})} \right]. \tag{9}$$

The whole computation reduces to the discussion of the solution of the saddle points equations,

$$q_{a_1 \ldots a_p} = 2g_p \langle\!\langle e^{-i(\lambda_{a_1} + \ldots + \lambda_{a_p})} \rangle\!\rangle \tag{10}$$

where the double brackets means the average over the one site partition function $\mathscr{Z}$.

In the spin-glass case the discussion of the saddlepoint solutions follows in a straightforward manner, even in the case of replica symmetry breaking. Now the problem is more involved due to the presence of a family of matrices parametrized by a finite number (from 1 to n) of indices, not just two as in the spin-glass case. In fact it is not obvious which is the breaking pattern. If we restrict ourselves, however, to the symmetric solution we can solve the saddlepoint equations in a simple way; in fact, we have only one parameter q, independent of any index.

This replica symmetric solution was studied some years ago (see reprints in [2]) and we also know its corrections to order $1/N$. Recently an extensive numerical analysis of this problem was presented [3] showing that the theoretical analysis done by Mézard and Parisi was really precise. There were obtained the analytical values of the asymptotic lengths inside 0.2% of the numerical simulation. It is also the first time that a replica prediction has been tested to such high precision. This gives us confidence to test the reality of the replica symmetry-breaking ansatz, a question left aside in [3].

To this end we can calculate analytically the probability distribution for the overlaps of the system, defined by

$$P(q) = \overline{\left\langle \delta \left(q - \frac{1}{N} \sum_{i<j} n_{ij} n'_{ij} \right) \right\rangle_{(2)}} \tag{11}$$

where $\langle\!\langle \cdot \rangle\!\rangle_{(2)}$ means the thermodynamical average over two real non-interacting identical copies of the system (i.e. with the Boltzmann weight $\prod_{ij} (T_{ij})^{n_{ij}} \prod_{lm} (T_{lm})^{n_{lm}}$ and with the same distribution of the lengths of the links). It is easy to calculate it directly, and for $\beta = \infty$, we get

$$P(q) = \delta(q(\beta = \infty) - 1). \tag{12}$$

This behaviour is typical for a system which is not in the spin-glass phase and the challenge is to test with a numerical simulation if this is the real behaviour for random matchings. If not, we should find, in the thermodynamical limit, a continuous part for $P(q)$ that extends down to zero overlap as in the SK model [2].

3. Numerical analysis

From the above it is clear that we are interested in the behaviour of the system at zero 'temperature'. We can take two roads; the first is to use some kind of annealing procedures, trying to be careful near the transition point, and then extrapolate the results down to zero 'temperature'. The second road is made possible by the combinatorial nature of the matching problems and seems the most natural and reliable one. We have obviously chosen the second and this numerical simulation makes use of the same routines [6] of our previous work [3] to which we address the reader for more information.

Our goal is to show the behaviour of $P(q)$ and for that purpose we need two different configurations of the same system. The configuration space for matching problems consists of a unit hypercube in $2N$ dimensions whose vertices are labelled by the configurations $\{n_{ij}\}$ of the feasible solutions. The algorithm we use will give us only the optimal (ground state) solution of the problem, so we have to find a technique to get new configurations from phase space that minimize the energy at zero 'temperature',

$$E(\beta = \infty) = \frac{1}{N} \sum_{i<j} n_{ij} l_{ij} \tag{13}$$

with the constraint of (3).

Fortunately, in combinatorial optimization, this technique is well known and goes under the name of post-optimal analysis. For matching problems the simplest technique is to choose one configuration $\{n_{ij}\}$, usually the optimal one, and then by fixing to a very large value, namely infinity, one of its links we solve from scratch [9] this new problem obtaining an *a priori* new configuration $\{n'_{ij}\}$. This is then used to calculate the overlap through

$$q = \frac{1}{N} \sum_{i<j} n_{ij} n'_{ij}. \tag{14}$$

It is then easy to follow this pattern and to generate other configurations and to calculate new overlaps with which we formed the histograms whose results are shown in the figures 2 and 4, which represent the bbehaviour for, respectively, simple matching with $r = 0$ and $r = 1$† (for all the simulations we take $N = 20, 50, 100, 200$ points with, respectively, 1000, 500, 300, 200 samples). They are in agreement in the thermodynamical limit, with the ansatz whose result is shown in (12). In fact, it is evident that they lack the continuous part which is present in the form of $P(q)$ and is the main feature of the reality of a broken replica-symmetry solution. It seems, therefore, that in the random matching problems the symmetrical ansatz is correct.

To be sure that we are correctly sampling the configuration space, we look for the difference between the energy per site of the ground state E_{GS} and that of the 'excited' one, E_{EXC}. We know from the theory of spin-glass that down to zero temperature there are, at least, two possible behaviours,

$$E_{EXC} - E_{GS} \approx O(1/N) \tag{15}$$

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† The sharp peaks in the figures are due to the integer discretization of the overlaps. The behaviour for the bipartite case is very similar.
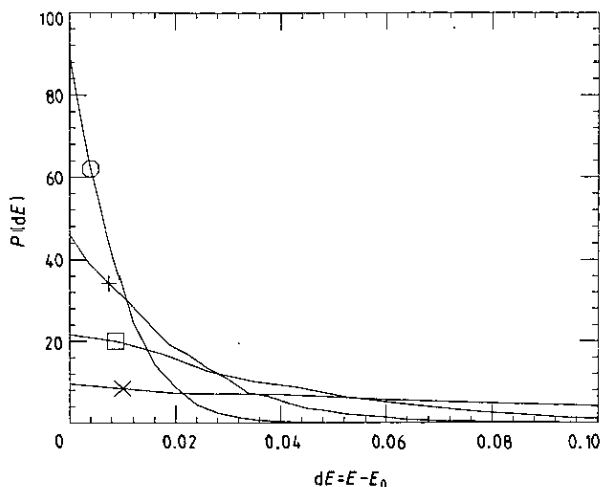
Figure 1. Distribution of the differences of energy between the ground state $E_{GS} = E_0$ and the excited states $E_{EXC} = E$ for the $r = 0$ simple matching case. $\bigcirc$, $N = 200$; $+$, $N = 100$; $\square$, $N = 50$; $\times$, $N = 20$.
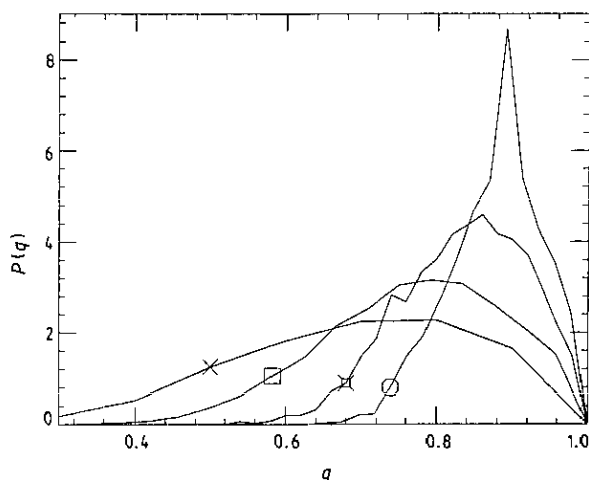

Figure 2. Probability distribution of the overlaps for the $r = 0$ simple matching case. Symbols as in figure 1.

or, otherwise,

$$E_{EXC} - E_{GS} \approx O(1) \tag{16}$$

corresponding to pure states in the first case and to metastable states in the second.

If post-optimal analysis leads us to possible candidates for new pure states, we expect to find the first behaviour for the energies of the excited states. This difference, together with the progressive sharpness of the $P(q)$, confirms that the number of stable configurations with nearest energy to the ground state, and overlap with it laying inside the tail of the $P(q)$, decrease as we go towards the thermodynamical limit. This seems to indicate that we have, with zero probability in the thermodynamical limit, optimal configurations with overlaps with the ground state different from $q = 1$. In other words, as N goes to infinity, 'excited' states concide with the ground state.
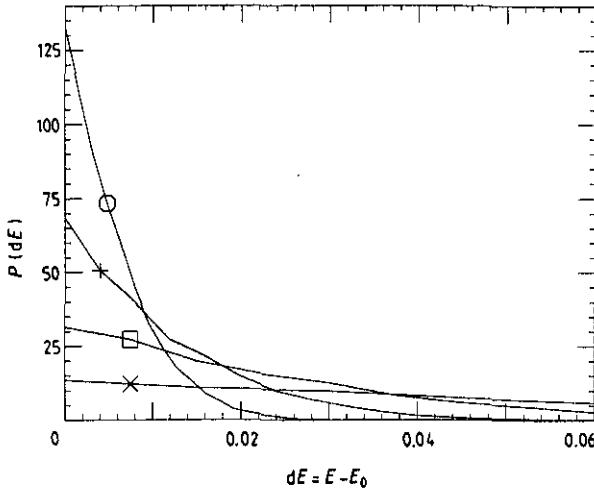
Figure 3. Distribution of the differences of enegy between the ground state $E_{GS} = E_0$ and the excited states $E_{EXC} = E$ for the $r = 1$ simple matching case. Symbols as in figure 1.
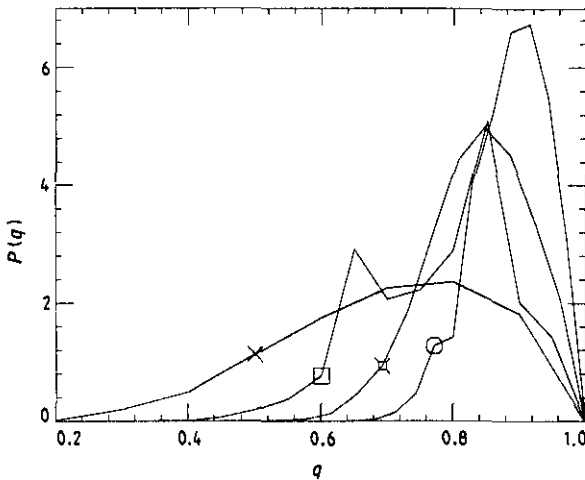

Figure 4. Probability distribution of the overlaps for the $r = 1$ simple matching case. Symbols as in figure 1.

The result of the simulations are showed in figures 1 and 3 (which represent the behaviour for, respectively, simple matching with $r = 0$ and $r = 1$†) and, once again, show agreement with our expectation, i.e., they are distributed as rapidly size-growing functions whose maximum at zero give us confidence on a good sampling of 'excited' states.

4. Conclusions

We present a large numerical simulation of random weighted matching problems by dealing with the nature of the replica symmetry. The simulation is in agreement with

† The same has been obtained for bipartite matching.

the absence of the breaking, as suspected earlier [3], by showing, mainly, the behaviour of the distribution of probability for the overlap, $P(q)$. One can speculate about the connection between the algorithmic complexity and the triviality of the phase space.

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