Chapter 1 Interpolation and Comparison Methods in the Mean Field Spin Glass Model

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Abstract We give a short overview of the recent rigorous mathematical methods developed for the study of complex disordered systems, in particular spin glasses in the mean field Sherrington-Kirkpatrick formulation. We show that interpolation methods, and related comparison arguments, are very powerful tools in order to study these models. We consider the problem of the infinite volume limit for the free energy, Then we introduce the Parisi solution for the spin glass, based on the spontaneous breaking of replica symmetry, and characterized by a functional order parameter entering in a variational principle. We show how the validity of the Parisi representation can be rigorously established. Finally, we point out some perspective for future developments.

1.1 Introduction

In a famous paper on Physical Review Letters, more than 30 years ago, David Sherrington and Scott Kirkpatrick introduced a celebrated mean field model for spin glasses [1,2], then considered to be a "solvable model".

The impact of this model on the theoretical physics research has been impressive. During the three decades after its introduction, hundreds and hundreds of papers have been devoted to the study of its properties, even through numerical methods.

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The relevance of the model surely comes from the fact that it is able to represent successfully, at least at the level of the mean field approximation, some important features of the physical spin glass systems, of great interest for their peculiar properties.

Some dilute magnetic alloys called spin glasses (see [3] and [4] for extensive reviews) are extremely interesting systems from a physical point of view. Their peculiar feature is to exhibit a new magnetic phase, where magnetic moments are frozen into disordered equilibrium orientations, without any long-range order. Moreover, these materials have some very slowly relaxing modes, with consequent memory effects.

The Sherrington-Kirkpatrick (SK) model is a simplified mean field model, intended to capture some basic properties of spin glasses.

There is also an additional very important reason for the relevance of this model, and related ones. In fact, recently it has become progressively clear that disordered systems of the Sherrington-Kirkpatrick type, and their generalizations, seem to play a very important role for theoretical and practical applications to hard optimization problems, as it is shown for example by Marc Mézard, Giorgio Parisi and Riccardo Zecchina in [5].

It is interesting to remark that the original paper was entitled "Solvable Model of a Spin-Glass", while a previous draft, according to what reported by David Sherrington, contained even the stronger denomination "Exactly Solvable". However, it turned out that the very natural solution devised by the authors is valid only at high temperatures, or for large external magnetic fields. At low temperatures, the proposed solution exhibits a nonphysical drawback given by a negative entropy, as properly recognized by the authors in their very first paper.

It took a few years to find an acceptable solution. This was done by Giorgio Parisi in a series of papers, by marking a radical departure from the previous methods. In fact, a very deep method of "spontaneous replica symmetry breaking" was developed. As a consequence the physical content of the theory was encoded in a functional order parameter of new type, and a remarkable structure began to show up for the pure states of the theory, characterized by a kind of hierarchical, ultrametric organization. These very interesting developments, due to Giorgio Parisi, and his coworkers, are explained in a challenging way in the classical book [6]. Part of this structure will be recalled in the following.

It is important to remark that the Parisi solution is presented in the form of an ingenious and clever *Ansatz*. Until a few years ago it was not known whether this *Ansatz* would give the true solution for the model, in the so-called thermodynamic limit, when the size of the system becomes infinite, or it would be only a very good approximation to the true solution.

The general structures offered by the Parisi solution, and their possible generalizations for similar models, exhibit an extremely rich and interesting mathematical content. In a very significant way, Michel Talagrand inserted a strongly suggestive sentence in the title to his book [7]: "Spin glasses: a challenge for mathematicians". As a matter of fact, the problem of giving a proper mathematical understanding of the spin glass structure is extremely difficult. In this talk, we would like to recall the main features of a very powerful method, yet extremely simple in its very essence, based on comparison and interpolation arguments on families of Gaussian random variables.

The method found its first simple application in [8], where it was shown that the Sherrington-Kirkpatrick replica symmetric approximate solution is a rigorous lower bound for the quenched free energy of the system, uniformly in the size, for any value of the temperature and the external magnetic field. Then, it was possible to reach a long awaited result [9]: the convergence of the free energy density in the thermodynamic limit.

Moreover, still by a generalized interpolation on families of Gaussian random variables, the first mentioned result, on the replica symmetric solution, was extended to give a rigorous proof that the expression given by the Parisi *Ansatz* is also a lower bound for the quenched free energy of the system, uniformly in the size [10]. The method gives not only the bound, but also the explicit form of the correction terms in the form of a sum rule. In a subsequent very important result, Michel Talagrand has been able to dominate these correction terms, showing that they vanish in the thermodynamic limit. This extraordinary achievement was firstly announced in a short note [11], containing only a synthetic sketch of the proof, and then presented with all details in a long paper in Annals of Mathematics [12].

The interpolation method is also at the basis of the far-reaching generalized variational principle proven by Michael Aizenman, Robert Sims and Shannon Starr in [13].

In this lecture, we will concentrate mostly on the main questions connected with the free energy. In particular, we will consider the subadditivity of the quenched free energy with respect to the system size, the existence of the infinite-volume limit, the broken replica symmetry sum rules and bounds, and the Parisi variational principle. Our treatment will be as simple as possible, by relying on the basic structural properties, and by describing methods of presumably very long lasting power.

The organization of the paper is as follows. In Sect. 1.2 we explain the basic features of the mean field spin glass models, by introducing all necessary definitions. In next Sect. 1.3 we give a simple application of the interpolation method to the mean-field spin glass model, by showing the sub-additivity of the quenched free energy with respect to the system size, and the existence of the infinite-volume limit [9].

Section 1.4 is devoted to a description of the main features of the Parisi representation for the free energy and to its rigorous establishment.

Section 1.5 is devoted to some results, which have been obtained after the talk given at INdAM, and to perspectives for further developments.

In conclusion, the author would like to thank the organizers of the first 2004 INdAM Day in Rome, in particular Corrado De Concini, for the kind invitation and exquisite hospitality.

1.2 Basic Definitions for the Mean Field Spin Glass Model

The generic configuration of the mean field spin glass model is defined through Ising spin variables $\sigma_i = \pm 1$, attached to each site i = 1, 2, ..., N.

But now there is also an external quenched disorder given by the N(N-1)/2independent and identical distributed random variables J_{ij} , defined for each couple of sites. For the sake of simplicity, we assume each J_{ij} to be a centered unit Gaussian with averages $E(J_{ij}) = 0$, $E(J_{ij}^2) = 1$. By quenched disorder we mean that the J have a kind of stochastic external influence on the system, without participating to the thermal equilibrium.

Now the Hamiltonian of the model is given by the mean field expression

$$H_N(\sigma, J) = -\frac{1}{\sqrt{N}} \sum_{(i,j)} J_{ij} \sigma_i \sigma_j.$$
(1.1)

Here, the sum runs over all couples of sites. Notice that the term \sqrt{N} is necessary in order to ensure a good thermodynamic behavior to the free energy, extensive in the system size N. For the sake of simplicity, we have considered only the case of zero external field. But the general case, with a magnetic external field, can be treated without any essential additional complication.

For a given inverse temperature β , let us now introduce the disorder-dependent partition function $Z_N(\beta, J)$ and the quenched average of the free energy per site $f_N(\beta)$, according to the definitions

$$Z_N(\beta, J) = \sum_{\sigma_1...\sigma_N} \exp(-\beta H_N(\sigma, J)), \qquad (1.2)$$

$$-\beta f_N(\beta) = N^{-1} E \log Z_N(\beta, J).$$
(1.3)

Notice that in (1.3) the average *E* with respect to the external noise is made *after* the log is taken. This procedure is called quenched averaging. It represents the physical idea that the external noise does not participate in the thermal equilibrium. Only the σ_i variables are thermalized.

For the sake of simplicity, it is also convenient to write the partition function in the following equivalent form. First of all let us introduce a family of centered Gaussian random variables $\mathcal{K}(\sigma)$, indexed by the configurations σ , and characterized by the covariances

$$E(\mathcal{K}(\sigma)\mathcal{K}(\sigma')) = q^2(\sigma, \sigma'), \qquad (1.4)$$

where $q(\sigma, \sigma')$ are the overlaps between two generic configurations, defined by

$$q(\sigma, \sigma') = N^{-1} \sum_{i} \sigma_i \sigma'_i, \qquad (1.5)$$

with the obvious bounds $-1 \le q(\sigma, \sigma') \le 1$, and the normalization $q(\sigma, \sigma) = 1$. Then, starting from the definition (1.1), it is immediately seen that the partition function in (1.2) can be also written, by neglecting unessential constant terms, in the form

$$Z_N(\beta, \mathcal{K}) = \sum_{\sigma_1...\sigma_N} \exp(\beta \sqrt{\frac{N}{2}} \mathcal{K}(\sigma)), \qquad (1.6)$$

which will be the starting point of our treatment. Here the dependence of the partition function on the random variables \mathcal{K} has been stressed in the notation.

According to the general well established strategy of statistical mechanics [14], firstly we consider the problem of the infinite volume limit.

1.3 The Thermodynamic Limit for the Free Energy

The proof of the convergence of the free energy per site in the thermodynamic limit was a result long awaited since decades. In [9] it was possible to give an unexpected very simple proof. Let us show the argument. Consider a system of size N and two smaller systems of sizes N_1 and N_2 respectively, with $N = N_1 + N_2$. Let us now compare

$$E \log Z_N(\beta, \mathcal{K}) = E \log \sum_{\sigma_1 \dots \sigma_N} \exp(\beta \sqrt{\frac{N}{2}} \mathcal{K}(\sigma)), \qquad (1.7)$$

with

$$E \log \sum_{\sigma_1...\sigma_N} \exp(\beta \sqrt{\frac{N_1}{2}} \mathcal{K}_1(\sigma^{(1)})) \exp(\beta \sqrt{\frac{N_2}{2}} \mathcal{K}_2(\sigma^{(2)})) = E \log Z_{N_1}(\beta, \mathcal{K}_1) + E \log Z_{N_2}(\beta, \mathcal{K}_2),$$
(1.8)

where $\sigma^{(1)}$ are the $(\sigma_i, i = 1, ..., N_1)$, and $\sigma^{(2)}$ are the $(\sigma_i, i = N_1 + 1, ..., N)$. Covariances for \mathcal{K}_1 and \mathcal{K}_2 are expressed as in (1.4), but now the overlaps are replaced with the partial overlaps of the first and second block, q_1 and q_2 respectively, defined as

$$q_1(\sigma, \sigma') = N_1^{-1} \sum_{i=1}^{N_1} \sigma_i \sigma'_i,$$
(1.9)

and analogously for the q_2 of the second block.

The key idea now is to build an interpolation scheme, between the large system and the two small systems. This is easily achieved by introducing the interpolation parameter $0 \le t \le 1$, and the interpolating auxiliary function $\phi(t)$, defined as

$$\phi(t) = E \log \sum_{\sigma_1 \dots \sigma_N} \exp(\sqrt{t}\beta \sqrt{\frac{N}{2}}\mathcal{K} + \sqrt{1-t}\beta \sqrt{\frac{N_1}{2}}\mathcal{K}_1 + \sqrt{1-t}\beta \sqrt{\frac{N_2}{2}}\mathcal{K}_2).$$
(1.10)

Here, we have realized the families of random variables $\mathcal{K}, \mathcal{K}_1, \mathcal{K}_2$ as independent on the same probability space. The interpolation through the \sqrt{t} and $\sqrt{1-t}$ assures a linear interpolation between the respective covariances. Obviously, we have

$$\phi(1) = E \log Z_N(\beta, \mathcal{K}),$$

while

$$\phi(0) = E \log Z_{N_1}(\beta, \mathcal{K}_1) + E \log Z_{N_2}(\beta, \mathcal{K}_2).$$

Now it is easy to calculate directly the *t* derivative of ϕ (see for example [15]), with the result

$$\frac{d}{dt}\phi(t) = \frac{\beta^2}{4} \frac{N_1 N_2}{N} \langle (q_1 - q_2)^2 \rangle_t, \qquad (1.11)$$

where $\langle \rangle_t$ is a quite complicated, but explicitly given, t dependent probability measure on the random variables (q_1, q_2) [15]. In this derivation we have exploited the simple connection between the global overlap and the block overlaps

$$Nq = N_1 q_1 + N_2 q_2. (1.12)$$

Since in any case the square in (1.11) is positive, by integrating on t and by exploiting the recognized boundary values at t = 0 and t = 1, we reach the super-additivity property

$$E \log Z_N(\beta, \mathcal{K}) \ge E \log Z_{N_1}(\beta, \mathcal{K}_1) + E \log Z_{N_2}(\beta, \mathcal{K}_2), \qquad (1.13)$$

firstly established in [9]. Of course, the corresponding free energies show a subadditive property, because of the minus sign involved in their definition.

From the superaddivity property, through standard methods [14], the existence of the limit follows in the form

$$\lim_{N \to \infty} N^{-1} E \log Z_N(\beta, \mathcal{K}) = \sup_N N^{-1} E \log Z_N(\beta, h, \mathcal{K}) \equiv -\beta f(\beta).$$
(1.14)

1.4 Comparison with the Parisi Representation for the Free Energy

We refer to the original paper [16], and to the extensive review given in [6], for the general motivations, and the derivation of the broken replica symmetry *Ansatz*, in the frame of the ingenious replica trick. Here we limit ourselves to a synthetic description of its general structure, independently from the replica trick. The deep motivation for the introduction of the Parisi trial functional is sketched in [17], in the frame of the cavity method (see also [18]).

First of all, let us introduce the convex space \mathcal{X} of the functional order parameters x, as nondecreasing functions of the auxiliary variable q, both x and q taking values on the interval [0, 1], i.e.

$$\mathcal{X} \ni x : [0, 1] \ni q \to x(q) \in [0, 1].$$
 (1.15)

Notice that we call x the function, and x(q) its values. We introduce a metric on \mathcal{X} through the $L^1([0, 1], dq)$ norm, where dq is the Lebesgue measure.

For our purposes, we will consider the case of piecewise constant functional order parameters, characterized by an integer *K*, and two sequences q_0, q_1, \ldots, q_K , m_1, m_2, \ldots, m_K of numbers satisfying

$$0 = q_0 \le q_1 \le \dots \le q_{K-1} \le q_K = 1, \ 0 \le m_1 \le m_2 \le \dots \le m_K \le 1, \ (1.16)$$

such that

$$x(q) = m_1 \text{ for } 0 = q_0 \le q < q_1, \ x(q) = m_2 \text{ for } q_1 \le q < q_2,$$

..., $x(q) = m_K \text{ for } q_{K-1} \le q \le q_K.$ (1.17)

In the following, we will find it convenient to define also $m_0 \equiv 0$, and $m_{K+1} \equiv 1$. The replica symmetric case of Sherrington and Kirkpatrick corresponds to

$$K = 2, q_1 = \bar{q}, m_1 = 0, m_2 = 1.$$
 (1.18)

Let us now introduce the function f, with values $f(q, y; x, \beta)$, of the variables $q \in [0, 1], y \in R$, depending also on the functional order parameter x, and on the inverse temperature β , defined as the solution of the nonlinear antiparabolic equation

$$(\partial_q f)(q, y) + \frac{1}{2}(\partial_y^2 f)(q, y) + \frac{1}{2}x(q)(\partial_y f)^2(q, y) = 0,$$
(1.19)

with final condition

$$f(1, y) = \log \cosh(\beta y). \tag{1.20}$$

Here, we have stressed only the dependence of f on q and y.

It is very simple to integrate Eq. (1.19) when x is piecewise constant. In fact, consider $x(q) = m_a$, for $q_{a-1} \le q \le q_a$, firstly with $m_a > 0$. Then, it is immediately seen that the correct solution of Eq. (1.19) in this interval, with the right final boundary condition at $q = q_a$, is given by

$$f(q, y) = \frac{1}{m_a} \log \int \exp(m_a f(q_a, y + z\sqrt{q_a - q})) d\mu(z),$$
(1.21)

where $d\mu(z)$ is the centered unit Gaussian measure on the real line. On the other hand, if $m_a = 0$, then (1.19) loses the nonlinear part and the solution is given by

$$f(q, y) = \int f(q_a, y + z\sqrt{q_a - q}) \, d\mu(z), \qquad (1.22)$$

which can be seen also to follow from (1.21) in the limit $m_a \rightarrow 0$. Starting from the last interval K, and using (1.21) iteratively on each interval, we easily get the solution of (1.19) and (1.20), in the case of piecewise constant order parameter x, as in (1.17), through a chain of Gaussian integrations.

Now we introduce the following important definitions. The trial auxiliary function, associated to a given mean field spin glass system, as described in Sect. 1.3, depending on the functional order parameter x, is defined as

$$\log 2 + f(0,0;x,\beta) - \frac{\beta^2}{2} \int_0^1 q \, x(q) \, dq.$$
 (1.23)

Notice that in this expression the function f appears evaluated at q = 0, and y = 0.

The Parisi spontaneously broken replica symmetry expression for the free energy is given by the definition

$$-\beta f_P(\beta) \equiv \inf_x \left(\log 2 + f(0,0;x,\beta) - \frac{\beta^2}{2} \int_0^1 q \, x(q) \, dq \right), \tag{1.24}$$

where the infimum is taken with respect to all functional order parameters x.

Notice that the infimum appears here, as compared to the supremum that would appear in a variational principle of the usual entropy type in statistical mechanics. Therefore, Parisi variational principle is really a new structure in statistical mechanics, that deserves careful study in itself.

In [10], by exploiting a suitable interpolation scheme, we have established a rigorous connection between the partition function of the mean field spin glass and the Parisi *Ansatz*. We skip all details and state only the final result, in the form of the sum rule

$$\log 2 + f(0,0;x,\beta) - \frac{\beta^2}{2} \int_0^1 q \, x(q) \, dq =$$
$$N^{-1} E \log Z_N(\beta,\mathcal{K}) + \frac{\beta^2}{4} \langle (q_{12} - q_a)^2 \rangle, \tag{1.25}$$

where $\langle \rangle$ is an explicitly given but quite complicated measure average over the variables σ , σ' , appearing in the two replica overlap q_{12} , and the variable $q_{.}$, taking the values q_a . The sum rule holds for any value of the order parameter x. One of the miracles occurring in the proof of this sum rule is that the second term appearing in the Parisi trial functional here comes for free from the completion of the square in the third term of the sum rule.

In any case, the third term, being the average of a square, is positive. Therefore we have the following important result.

Theorem 1.1. For all values of the inverse temperature β , and for any functional order parameter *x*, the following bound holds

$$N^{-1}E\log Z_N(\beta, \mathcal{K}) \le \log 2 + f(0, 0; x, \beta) - \frac{\beta^2}{2} \int_0^1 q \, x(q) \, dq,$$

uniformly in N. Consequently, we have also

$$N^{-1}E\log Z_N(\beta, \mathcal{K}) \le \inf_x (\log 2 + f(0, h; x, \beta) - \frac{\beta^2}{2} \int_0^1 q \, x(q) \, dq),$$

uniformly in N.

This result can be understood also in the frame of the generalized variational principle established by Aizenman-Sims-Starr [13], as shown for example in [15], by exploiting the general structure of the Derrida-Ruelle-Parisi probabibility cascades.

Up to this point we have seen how to obtain upper bounds. The problem arises whether we can also get lower bounds, so as to shrink the thermodynamic limit to the value given by the \inf_x in Theorem 1.1. After a short announcement in [11], Michel Talagrand wrote an extended paper [12], where the complete proof of the control of the lower bound is firmly established. We refer to the original paper for the complete details of this remarkable achievement. About the methods, here we only recall that the sum rule in [10], explained above, gives also the corrections to the bounds appearing in Theorem 1.1, albeit in a quite complicated form. Talagrand has been able to establish that these corrections do in fact vanish in the thermodynamic limit. In order to be able to reach this important result it is necessary to prove an extension of the broken replica symmetry bounds of Theorem 1.1 to the case where two replicas of the system are coupled together. This task has not been reached yet in its full generality, but the treatment given by Talagrand is sufficient to prove the vanishing of the correction terms in the infinite volume limit.

In conclusion, we can establish the following conclusive result about the expression of the free energy in the mean field spin glass.

Theorem 1.2. For the mean field spin glass model we have

$$\lim_{N \to \infty} N^{-1} E \log Z_N(\beta, \mathcal{K}) = \sup_N N^{-1} E \log Z_N(\beta, \mathcal{K})$$
(1.26)

$$= \inf_{x} \left(\log 2 + f(0,0;x,\beta) - \frac{\beta^2}{2} \int_0^1 q \, x(q) \, dq \right). \tag{1.27}$$

1.5 Further Developments and Outlook

As we have seen, in these last few years there has been an impressive progress in the understanding of the mathematical structure of spin glass models, mainly due to the systematic exploitation of interpolation methods. However many important problems are still open. The most important one is the full understanding of the hierarchical ultrametric organization of the overlap distributions, as appears in Parisi theory, and the decomposition in pure states of the glassy phase, at low temperatures. An important step in this direction have been obtained through the establishment of the so called Ghirlanda-Guerra identities [19]. Based on these, Dmitry Panchenko [20] has been able to prove ultra-metricity of the overlap distribution, a very remarkable achievement of the last years.

Moreover, interpolation and comparison methods have been extended to other important disordered models, such as for example neural networks, bipartite models, multi-species models. Here the difficulty is that the positivity arguments, so essential in the application of the interpolation methods, do not seem to emerge naturally inside the structure of the theory. For recent results see [21-27].

Even for a class of simple mean field diluted ferromagnetic systems, the treatment of the infinite volume limit has not been reached yet, due to the lack of positivity arguments. Only the $\beta \rightarrow \infty$ limit is well understood [28].

For extensions to diluted spin glass models we refer for example to [29–31].

Finally, the problem of connecting properties of the short-range model with those arising in the mean field case is still almost completely open. For partial results, and different points of view, see [32–37].

Finally, we mention a pedagogically very useful complete review appeared [38], about the application of the interpolation methods, and the other methods of spin glass theory, to the simple case of the ferromagnetic mean field model.

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