PhD Project

The Parisi formula and beyond: A PDE approach to disordered systems

The goal of this project is to study the global properties of large collections of units that interact in a disordered manner. This setting encompasses many models of interest arising in a diversity of areas such as combinatorics, computer science, statistics, or high-dimensional geometry. Notable examples include random constraint satisfaction problems [37, 36, 30, 33, 18, 20], the random assignment and traveling salesman problems [34, 3, 4], community detection and more general problems of large-scale statistical learning [1, 65], error correcting codes in information theory [53], and combinatorial problems such as graph coloring [42, 19, 13]. This proposal places particular emphasis on problems that relate to statistical learning and the modeling of neural networks. Prominent models in the latter setting include the perceptron model [32] and restricted Boltzmann machines [55, 27], which are usually considered in the statistical context of classification tasks, and the Hopfield model [31, 28], which is usually thought of as a neural model of memory storage and retrieval.

Scientific Context and Motivations

The situations mentioned above can be thought of as large-scale optimization problems that are inherently "complex" and difficult to solve. While spectacular progress has been achieved in the simplest settings such as for the Sherrington-Kirkpatrick (or SK) model, even modest generalizations of this model remain poorly understood. The SK model, defined precisely below, is a "completely mean-field" model in which all units are exchangeable. If we depart slightly from this assumption and assume instead, for instance, that the elementary units are organized over two layers, with direct interactions going only from one layer to another, then most techniques break down and our understanding becomes extremely limited. This two-layer organization can be thought of as a purely random realization of a simple artificial neural network called a restricted Boltzmann machine, and a number of fascinating predictions have been put forward in [64] by relying on this connection. This proposal aims to make fundamental progress on the theoretical analysis of a number of facets of a general class of models that contains two- and multi-layer models as special cases.

We will start by discussing the SK model and its key properties more precisely. The SK model is defined as follows [54]. There are N units in the system, labeled $1, ..., N$. We can think of these units as representing people, which we are tasked to split into two groups; a splitting can be represented by a vector $\sigma \in \{-1, 1\}^N$, with the understanding that $\sigma_i = \sigma_j$ if and only if the individuals i and j are assigned to the same group. We are also given a family $(J_{ij})_{1\le i,j\le N}$ of coefficients that represent the "quality" of the interaction between i and j, with $J_{ij} > 0$ if i and j get along well with each other, and $J_{ij} < 0$ otherwise. We would like to find a group assignment that maximizes the sum total of the interaction qualities within each group. This is equivalent to the problem of maximizing the function

$$H_N(\sigma) = \frac{1}{\sqrt{N}} \sum_{1\le i,j\le N} J_{ij}\sigma_i\sigma_j, \ \sigma \in \{-1, 1\}^N \tag{1}$$

(We write $\sigma_i\sigma_j$ here instead of the possibly more natural choice of $\mathbf{1}_{\sigma_i=\sigma_j}$ for historical reasons having to do with the modeling of magnetic materials; since $\mathbf{1}_{\sigma_i=\sigma_j} = \frac{1}{2}\big(\sigma_i\sigma_j + 1\big)$ this is harmless; the normalization term $\frac{1}{\sqrt{N}}$ will be useful later on.) Naturally, this problem will depend on what the coefficients (J_{ij}) look like. We ask here about properties of a typical such problem, by positing that the coefficients (J_{ij}) are sampled randomly beforehand as independent standard Gaussians. The idea of looking at random realizations allows us to probe objects that would otherwise defy our analytic abilities, and to avoid worst-case considerations that often lack practical relevance.

This optimization problem is “complex” in the sense that the identification of an optimizer for the function H_N is a difficult task. Indeed, if, say, the coefficients J_{12} and J_{13} are positive, but J_{23} is negative, then it will not be possible to find a configuration in which each of the summands in H_N takes its maximal value (the signs of J_{12} and J_{13} would suggest to enforce $\sigma_1 = \sigma_2 = \sigma_3$, while the sign of J_{23} would suggest to enforce $\sigma_2 = -\sigma_3$). In other words, the optimizer will retain frustrations. Relatedly, a naive greedy procedure that iteratively flips each coordinate σ_i one at a time whenever a flip brings about an increase of the value of H_N will typically not end up on an optimal configuration. In the original context of condensed matter physics where such models were introduced, the units σ_i are thought of as spins, and physicists qualify systems with frustrations as glassy. The SK model and its generalizations are therefore called spin glasses.

For physical and mathematical reasons, it is natural to consider the family of Gibbs measures associated with the energy function H_N. Indeed, if we think of σ as a collection of spins embedded in physical space, then they will be subject to external thermal noise. At inverse temperature $\beta \geq 0$, the Gibbs principle states that the probability to find the system in the configuration $\sigma \in \{-1, 1\}^N$ is proportional to $\exp(\beta H_N(\sigma))$. This notion of Gibbs measure allows us to smoothly interpolate between the uniform measure over $\{-1, 1\}^N$, obtained when $\beta = 0$, and measures which will concentrate more and more on the near-optimizers of H_N, as β tends to infinity. Notice that there are now two levels of randomness at play here: first we sample the coefficients (J_{ij}) randomly; and then the Gibbs measure is defined for each realization of these coefficients. We denote by $\mathbb{E}$ the expectation with respect to the variables (J_{ij}).

One of Giorgio Parisi’s most momentous breakthroughs [49, 48, 50, 52], recently celebrated by the 2021 Nobel prize in physics [51], is the discovery of a formula for the limit behavior of the free energy

$$F_N(\beta) = \frac{1}{N}\mathbb{E} \log \sum_{\sigma \in \{-1,1\}^N} \exp(\beta H_N(\sigma)) \tag{2}$$

The formula predicted by Parisi for the limit of F_N is relatively complicated, and its derivation involves very sophisticated and non-rigorous arguments, so much so that it was initially controversial in the physics community. With the combined efforts of several other physicists, it progressively became clear that this formula was indeed the correct solution [35]. In groundbreaking contributions, Parisi’s prediction received its definite confirmation when Francesco Guerra and Michel Talagrand gave it a rigorous proof [25, 60]; this proof was then revisited and extended in [43, 44].

To describe the class of models covered by the current techniques, it is useful to focus on the covariance structure of the function H_N : for every $\sigma, \tau \in \{-1, 1\}^N$, we have :

$$\mathbb{E}[H_N(\sigma)H_N(\tau)] = N\xi\left(\frac{\sigma \cdot \tau}{N}\right) \tag{3}$$

where $\sigma \cdot \tau$ is the scalar product between σ and τ , and $\xi(r) = r^2$. More general models allow for a finite number D of types for the units, which we can encode as $(\sigma_{d,i})_{1\leq d\leq D, 1\leq i\leq N}$ (the length of each of the vectors σ_d could in principle depend on d as well), but we refrain from doing so to lighten the notation) . In order to retain a high degree of symmetry in the models, we ask that the covariance be expressed as a function ξ of the matrix of scalar products $(\frac{\sigma_d \cdot \sigma_{d'}}{N})_{1\leq d,d'\leq D}$. The models that are now relatively well-understood are those for which the function ξ is convex [26, 61, 14, 43, 44, 11, 45, 47, 46].

Many models of interest fall outside of this class. For instance, if the units are organized over two layers and only have direct interactions across layers (this case will henceforth be referred to as the bipartite model), then the covariance reads, for every $\sigma = (\sigma_1, \sigma_2), \tau = (\tau_1, \tau_2) \in \{-1, 1\}^N \times \{-1, 1\}^N$,

$$\mathbb{E}[H_N(\sigma)H_N(\tau)] = N\left(\frac{\sigma_1 \cdot \tau_1}{N}\right)\left(\frac{\sigma_2 \cdot \tau_2}{N}\right) \tag{4}$$

That is, the relevant function ξ in this case is $\xi(x_1, x_2) = x_1x_2$, which is not convex. As a result, the physicists’ predictions for this model become equivocal. To the best of my understanding, until my recent work [40], there was not even a fully precise prediction for what the limit free energy should be in this case. The mathematical understanding of this class of models therefore remains extremely limited.

Description of the project

The determination and analysis of the limit free energy allow for the identification of different regimes, or phases, separated by sharp transitions. Examples include identifying whether a large-scale constraint satisfaction problem admits a solution [33], whether one can recover non-trivial information from noisy data in statistical inference [9], whether data classification will be successful [65], how many patterns can be stored and retrieved by a memory model [62, 63], etc.

The natural possible generalizations of Parisi's variational formula to the bipartite model are false [40]. While physicists have relied on modified formulations based on fixed point equations [29, 22, 23], these equations do not have unique solutions in general, and are thus equivocal. Exploring a new approach, in [40] a clear conjecture for what the limit free energy should be has been presented, and the conjectural limit has been proved to be an upper bound to the true quantity. These results were then generalized to essentially any mean-field spin glass model in [39]. Showing the converse bound turns out to be much more challenging, one of the main goals of this proposal is to resolve this problem.

The approach we will study during this research project, partly inspired by [24, 10, 2, 12], rests on a new point of view based on the discovery that, in the limit of large system size, a suitable extension of the free energy solves a partial differential equation (PDE) of Hamilton-Jacobi type. Naturally, this point of view is consistent with known results: for the SK model and its close cousins, it was showed in [38, 41] that Parisi's formula can be reformulated as follows. Let $\mathcal{P}(\mathbb{R}_+)$ be the space of probability measures over $\mathbb{R}_+$, and let $f = f(t, \mu) : \mathbb{R}_+ \times \mathcal{P}(\mathbb{R}_+) \to \mathbb{R}$ be the solution to

$$\begin{cases} \partial_t f + \int \xi(\partial_\mu f) d\mu = 0 & \text{in } \mathbb{R}_+ \times \mathcal{P}(\mathbb{R}_+) \\ f(0, \cdot) = \psi & \text{in } \mathcal{P}(\mathbb{R}_+) \end{cases} \tag{5}$$

where ψ is a functional transform of the Bernoulli ± 1 measure named the "cascade transform" in [39], and where the function ξ appearing in (3)-(5) is $\xi(r) = r^2$ for the SK model. Then

$$\lim_{N\to\infty} \frac{1}{N} \mathbb{E} \log \sum_{\sigma \in \{-1,1\}^N} \exp(\sqrt{2t} H_N(\sigma) - Nt) = f(t, \delta_0). \tag{6}$$

The derivative $\partial_\mu f$ appearing in (5) is of transport type [5]. This approach to the description of the limit free energy is remarkably synthetic. For instance, for other models in which a more general convex function ξ appears in (3), the statement above remains valid without any modification. At least for finite-dimensional versions of equations of the form of (5), it is well-known that the solution can be expressed by a variational formula provided that the nonlinearity (here the function ξ) is convex [21]. A change of variables then allows one to relate this representation with Parisi's formula [38].

The situation changes radically for nonconvex ξ, such as for the bipartite model for which $\xi(x_1, x_2) = x_1 x_2$. On the one hand, Parisi's variational formula simply breaks down [40]. On the other hand, up to a simple adaptation of the definition of the PDE in (5) in which the variable μ is replaced by a pair (μ_1, μ_2), and $\xi(\partial_\mu f)$ is replaced by $\partial_{\mu_1} f \partial_{\mu_2} f$, the formulation above immediately suggests a plausible conjecture for the limit free energy in this case.

The justification of this conjecture is a long-term project that requires a combination of advanced probability and analysis techniques. In particular, the absence of convexity of the nonlinearity in the equation (5) mandates that we appeal to the notion of viscosity solutions [21]. One needs to identify new selection principles that allow to ascertain that a function is the viscosity solution from relatively weak assumptions. A promising selection principle was identified in [15], and allowed for the resolution of a very large class of problems of statistical inference. However, its assumptions are still too stringent in the context of spin-glass models.

If this can be achieved, the rich phenomenology of phase transitions will remain to be described. A first crucial point will be to show a transition of replica symmetry breaking for these more general models, which will now have to be read directly from PDE arguments. Connections with alternative points of view such as [16, 6, 7, 8, 17, 56, 58, 57, 59] will also be sought for.

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