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A Friendly Tutorial on Mean-Field Spin Glass Techniques for Non-Physicists

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A Friendly Tutorial on Mean-Field Spin Glass Techniques for Non-Physicists

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ABSTRACT

Mean-field spin glasses are a class of high-dimensional random cost (energy) function with special exchangeability properties. Random probability measures are defined from these energy functions by the usual Boltzmann formula. Over the last 40 years, an arsenal of sophisticated mathematical techniques (both rigorous and non-rigorous) has been developed to characterize these models. More recently, these techniques have been successfully applied to a number of canonical models in high-dimensional statistics and machine learning, which fit the same framework. This tutorial provides an introduction to such techniques, aimed at non-specialists.

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Introduction

I thought fit to write out for you and explain in detail in the same book the peculiarity of a certain method, by which it will be possible for you to get a start to enable you to investigate some of the problems in mathematics by means of mechanics. [...] it is of course easier, when we have previously acquired, by the method, some knowledge of the questions, to supply the proof than it is to find it without any previous knowledge.

—Archimedes, On the method

This tutorial is based on lecture notes written for a class taught in the Statistics Department at Stanford in the Winter Quarter of 2017 and then again in Fall 2021. The class was called “Methods From Statistical Physics (Stats 369)” and was addressed to students from Statistics, Mathematics, and Engineering Departments with a solid background in probability theory, but no previous knowledge of physics. The objective was to provide a working knowledge of some of the techniques developed over the last 40 years by theoretical physicists and mathematicians to study mean field spin glasses and their applications to high-dimensional statistics and statistical learning.

Why Mean Field Spin Glasses?

The history of the subject is truly remarkable.¹ Spin glass models were introduced by physicists in the 1970s to model the statistical properties of certain magnetic materials. Over the last half century, these models have motivated a blossoming line of mathematical work with applications to multiple fields, at first sight distant from physics.

From a mathematical point of view, spin glasses are high-dimensional probability distributions, i.e., probability distributions over \mathbb{R}^n , $n \gg 1$, which are usually written in the Gibbs–Boltzmann form

$$\mu(d\boldsymbol{\sigma}) \propto e^{\beta H(\boldsymbol{\sigma})} \nu_0(d\boldsymbol{\sigma}). \quad (1)$$

Here ν_0 is a “simple” reference measure (for instance the uniform distribution over $\{+1, -1\}^n$ or the uniform distribution over the sphere S^{n-1}), the exponential weight $H: \mathbb{R}^n \rightarrow \mathbb{R}$ is known as the Hamiltonian (the standard convention in physics is to refer to $-H$ as the Hamiltonian), and $\beta > 0$ is known as the inverse temperature.

Of course, any probability measure in \mathbb{R}^n can be written in the form (1). However in spin glass models, $H(\boldsymbol{\sigma})$ is typically a sum of polynomially many (in n) “simple” terms (e.g., low degree monomials in the coordinates σ_i), and hence the form (1) is meaningful. It is worth mentioning that, while we focus for simplicity on probability measures over \mathbb{R}^n , spin glass models have been studied in other product spaces \mathcal{X}^n as well.

In spin glass models, the Hamiltonian $H(\cdot)$ itself is random or, to be precise, $\{H(\boldsymbol{\sigma})\}_{\boldsymbol{\sigma} \in \mathbb{R}^n}$ is a stochastic process indexed by $\boldsymbol{\sigma} \in \mathbb{R}^n$ (or $\boldsymbol{\sigma} \in \Sigma$, where Σ denotes the support of ν_0). Therefore the measure $\mu(d\boldsymbol{\sigma})$ is a random probability measure. A specific spin glass model is defined by specifying the distribution of the process H (alongside the reference measure ν_0).

¹The reader interested in early historical overviews might wish to consult the sequence of seven expository articles written by Phil Anderson, between 1988 (Anderson, 1988) and 1990 (Anderson, 1990), or of course the unsurpassed collection of articles (and accompanying introductions) in Mézard *et al.* (1987). For a personal account, see Charbonneau (2021).

At first sight, studying random probability measures might seem a somewhat exotic endeavor. However, a little thought reveals that random probability measures are both ubiquitous and useful:

- (1) Consider a statistical estimation problem: we want to estimate an unknown vector $\boldsymbol{x} \in \mathbb{R}^n$ from some data \boldsymbol{Y} . We will see several examples of this problem in this tutorial. A Bayesian approach postulates a prior distribution over \boldsymbol{x} , and then forms a posterior, namely the conditional distribution of \boldsymbol{x} given \boldsymbol{Y} , under that prior. The posterior is a random probability distribution over \mathbb{R}^n (because \boldsymbol{Y} is random).
- (2) Consider an optimization problem of the form $\max_{\boldsymbol{\sigma} \in \Sigma} H(\boldsymbol{\sigma})$. In many circumstances, we have a probabilistic model for H . For instance, this is the case in empirical risk minimization, which is the standard approach to statistical learning. Of course, in order to understand the properties of this optimization problem, it is important to understand the geometry of the (random) superlevel sets $\Sigma_E := \{\boldsymbol{\sigma} \in \Sigma: H(\boldsymbol{\sigma}) \geq E\}$. It turns out that—in many cases—the distribution (1) is closely related to the uniform distribution over $\Sigma_{E(\beta)}$ for a certain $E(\beta)$. Therefore, the Gibbs measure (1) is a powerful tool to explore the random geometry of superlevel sets.
- (3) In physics, the Hamiltonian H is random because, for instance, the spins σ_i are magnetic moments associated to impurities at random locations in an otherwise non-magnetic material. More generally, H can be random because it is the Hamiltonian of a disordered system, whose “disorder” degrees of freedom are not thermalized.

Mean field spin glass models are a special subfamily of spin glass models. Roughly speaking, they are characterized by the fact that the coordinates of $\boldsymbol{\sigma}$ (the “spins” in physics language) are “indistinguishable” from the point of view of the process² $H(\cdot)$. The first model

²Formally, for any fixed number of vectors $\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_k$, the joint distribution of $(H(\boldsymbol{\sigma}_1), \dots, H(\boldsymbol{\sigma}_k))$ depends on $\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_k$ only through the joint empirical distribution of their coordinates $n^{-1} \sum_{i=1}^n \delta_{\sigma_{1,i}, \dots, \sigma_{k,i}}$.

of this type, which we will study in Section 2, was first introduced by David Sherrington and Scott Kirkpatrick in 1975 (Sherrington and Kirkpatrick, 1975) to provide an idealized model that could be amenable to mathematical analysis.

In the near half-century since then, and starting with the invention of “replica symmetry breaking” by Parisi (1979a), physicists have developed a number of sophisticated non-rigorous techniques to analyze mean field spin glasses and characterize their high-dimensional behavior. While several of the physicists’ results and technique are outstanding challenges for mathematicians, since the early 2000s, there has been increasing success in rigorizing some of these ideas. These developments have given birth to a rich and rapidly evolving area of probability theory.

In parallel with these developments, it has become increasingly clear that understanding the behavior of random high-dimensional probability distributions $\mu(d\boldsymbol{\sigma})$ and of random high-dimensional objective functions $H(\boldsymbol{\sigma})$ is crucial in a number of mathematical disciplines beyond theoretical physics. We mentioned above high-dimensional statistics and statistical learning: tools and intuitions from physics have found countless applications in these areas in the last 10–15 years. In the opposite direction, high-dimensional statistics and statistical learning have brought new questions and stimulated new developments in spin glass theory.

This tutorial is mainly aimed at researchers in statistics, mathematics, computer science, who want to learn some of the important tools and ideas in this area.

The Style of This Tutorial

This tutorial is deliberately written in a somewhat non-standard style, from several viewpoints:

Concrete problems. Rather than developing the theory in the most general setting, we focus on two concrete problems that are motivated by questions in statistical estimation. Each of the next two sections is dedicated to one such problem.

We use each of these examples as a pretext for presenting a number of mathematical techniques. We believe it is best to learn these technique on concrete applications.

Non-exhaustive. Our treatment is far from exhaustive, even for each of the specific problems that we treat. On the other hand, while we use these examples as motivation, we do not hesitate in pursuing detours that are interesting, but indirectly related to the original questions posed by those examples.

Rigorous vs. non-rigorous techniques. We present a mixture of non-rigorous and rigorous techniques. Whenever something is proven (or a proof in the literature is indicated, or sketched) we emphasize this by using the labels “theorem,” “lemma,” and so on. On the other hand, we explain non-rigorous techniques on examples for which rigorous alternatives (yielding the same conclusions) are available.

There are countless reasons for learning non-rigorous techniques in parallel with rigorous ones. Among others: (i) They have driven this research area; (ii) Properly used, they provide the correct answer with significantly less work; (iii) They apply more broadly; (iv) They can provide invaluable insights/conjectures for rigorous research.

As shown by the quote above, reason (iv) was already acknowledged by Archimedes more than two millennia ago.

Exercises. As explained above, this tutorial is based on a class taught at Stanford. We include the exercises developed for that class (often generalizations of the models treated in the main text). The importance of hands-on practice in mathematics cannot be overstated. Even more so when learning a completely different point of view (e.g., learning non-rigorous techniques for a mathematically minded person, or vice versa).

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