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Application of the maximum relative entropy method to the physics of ferromagnetic materials

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HIGHLIGHTS

- Probability distribution functions are approximated via maximum relative entropy methods.
- Numerical estimates of effective energy levels of atoms in defective ferromagnetic materials are presented.
- A maximum relative entropy method characterization of defective ferromagnetic materials is proposed.

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ABSTRACT

It is known that the Maximum relative Entropy (MrE) method can be used to both update and approximate probability distributions functions in statistical inference problems. In this manuscript, we apply the MrE method to infer magnetic properties of ferromagnetic materials. In addition to comparing our approach to more traditional methodologies based upon the Ising model and Mean Field Theory, we also test the effectiveness of the MrE method on conventionally unexplored ferromagnetic materials with *defects*.

1. Introduction

In 1957, Jaynes [1,2] showed that maximizing statistical mechanic entropy for the purpose of revealing how gas molecules were distributed was simply the maximizing of the Shannon information entropy [3] with statistical mechanical information. This idea lead to MaxEnt or his use of the Method of Maximum Entropy for assigning probabilities. This method has recently evolved to a more general method, the method of Maximum relative Entropy (MrE) [4] which has the advantage of not only assigning probabilities but *updating* them when new information is given in the form of constraints on the family of allowed posteriors. One of the drawbacks of the MaxEnt method was the inability to include data. When data was present, one used Bayesian methods. The methods were combined in such a way that MaxEnt was used for assigning a prior for Bayesian methods, as Bayesian methods could not deal with information in the form of constraints, such as expected values. Previously it has been shown that one can use the MrE method to reproduce a mean field solution for a simple fluid [5]. The purpose of this was to illustrate that in addition to updating probabilities, MrE can also be used for *approximating* probability distributions as an approximation tool.

In a simple ferromagnetic material (that is, a ferromagnetic material with a single domain), the electronic spins of the individual atoms are strong enough to affect one and other, and give rise to the so called exchange interaction [6]. This effect,

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however, is temperature dependent. When the temperature is below a certain point (the Curie or critical temperature) the spins tend to all point in the same direction due to their influence on each other. This establishes a permanent magnet as the individual atoms produce a net dipole effect. Above this temperature, the atoms cease to have a significant effect on each other and the material behaves more like a paramagnetic substance. Determining this net dipole effect can be difficult. First, the interactions are due to complicated quantum effects. Second, since a given material has a very large number of atoms, computing the net dipole effect can be difficult in two dimensions and completely intractable in three dimensions. Therefore, approximations such as using an Ising Model [7–9] and/or the mean field approximation [10–12] are made to facilitate computation.

Applications of the MrE (updating) method together with information geometric methods used to characterize the complexity of dynamical systems described in terms of probabilistic tools are quite extensive [13–21]. In Refs. [14,15], using the MrE method together with differential geometric techniques, we proposed an information-geometric characterization of chaotic energy level statistics of a quantum antiferromagnetic Ising spin chain in a tilted magnetic field. In Ref. [21], employing the very same aforementioned techniques, we were able to establish a connection between the behavior of the information-geometric complexity of a trivariate Gaussian statistical model and the geometric frustration phenomena that appears in triangular Ising models [22]. However, the purpose of our article is to illustrate the use of the MrE (approximating) method as a tool for attaining approximations for ferromagnetic materials that lie outside the ability of traditional methods. In doing so, we further the previous work done and show the versatility of the method.

The layout of the remaining part of this manuscript is as follows. In Section 2, we briefly outline the essential steps of the MrE method in updating and approximating probability distributions. In Section 3, we describe the basics of the Ising model and Mean Field Theory as approximate mathematical descriptions of ferromagnetic materials. In Section 4, we compare magnetization properties of ferromagnets inferred by means of MrE with those obtained via the Ising model together with Mean Field Theory. In Section 5, we further test the effectiveness of the MrE methodology by considering ferromagnetic material in the presence of defects. Our final remarks appear in Section 6.

2. The maximum relative entropy method

In this section, we outline the essential elements of the MrE method as a technique for updating and/or approximating probability distributions.

2.1. Updating probability distributions

The MrE method is a technique for updating probabilities when new information is provided in the form of a constraint on the family of the allowed posteriors. The main feature of the MrE method is the possibility of updating probabilities in the presence of both data and expected value constraints. This feature was first formally presented in Ref. [4] where, in particular, it was shown that Bayes updating can be regarded as a special case of the MrE method. A first semi-quantitative analysis of the effective advantages of this powerful feature of the MrE method appeared in Ref. [23]. Finally, the first fully quantitative investigation of the advantages of the MrE method was carried out in Ref. [24] where two toy problems were solved in detail. Following these lines of investigation, we present here a novel application of the MrE method to a real-world ferromagnetic problem.

We use the MrE method to update from a prior to a posterior probability distribution. Specifically, we want to make inferences on some quantity $\theta \in \Theta$ given:

(i) the prior information about θ (the prior);
(ii) the known relationship between $D \in \mathcal{D}$ and $\theta \in \Theta$ (the model);
(iii) the observed values of the variables (data) $D \in \mathcal{D}$.

The search space for the posterior probability distribution occurs in the product space $\mathcal{D} \times \Theta$, and the joint distribution is denoted as $P(D, \theta)$. The key idea is going from the old prior $P_{\text{old}}(\theta)$ to the updated prior $P_{\text{new}}(\theta)$,

$$P_{\text{new}}(\theta) \stackrel{\text{def}}{=} \int \mathrm{d}D P_{\text{new}}(D, \theta) \,. \tag{1}$$

The joint probability $P_{\text{new}}(D, \theta)$ maximizes the relative entropy functional $S[P|P_{\text{old}}]$,

$$S[P|P_{\text{old}}] \stackrel{\text{def}}{=} -\int \mathrm{d}D\mathrm{d}\theta P(D, \theta) \log\left[\frac{P(D, \theta)}{P_{\text{old}}(D, \theta)}\right], \tag{2}$$

subject to the given information constraints. Note that $P_{\text{old}}(D, \theta)$,

$$P_{\text{old}}(D, \theta) = P_{\text{old}}(D|\theta) P_{\text{old}}(\theta) \,, \tag{3}$$

is called here the joint prior, while $P_{\text{old}}(\theta)$ and $P_{\text{old}}(D|\theta)$ denote the standard Bayesian prior and the likelihood, respectively. We emphasize that both the joint prior and the standard Bayesian prior encode prior information about $\theta \in \Theta$. Furthermore, despite the fact that the likelihood is not regarded as prior information in the conventional sense, it will be considered here