
Theory and Methods for the Ferromagnetic Ising Model

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Abstract

The Ising model is a historically important problem in statistical mechanics. Although it was originally proposed as a crude approximation of ferromagnetic phenomena, it furnished statistical mechanics, and later probabilistic science as whole, with a new paradigm of graph-based modeling that would prove influential. Especially in the distilled, theoretical study of probabilistic graphical models (PGMs), which today is its own field, many methods developed for Ising models and spin-glasses have been repurposed and reinterpreted, as have the rich physical vocabulary of energies, entropy, and partition functions.

In this paper, we pay homage to the Ising model by applying modern methods to the original problem of ferromagnetism. We discuss the theory of the Ising model both from a PGMs and statistical mechanics point of view, examining the correspondence. We then evaluate a number of approaches to inference—Markov Chain Monte Carlo, belief propagation, and variational inference. Finally, we show the successes and limitations of the Ising model in the context of physical phenomena.

1 Theory of the Ising Model

A particle with magnetic moment $\vec{\mu}$ in an external magnetic field \vec{B} has potential energy:

$$U = -\vec{\mu} \cdot \vec{B}$$

A particle also creates an intrinsic magnetic field defined by magnetic moment $\vec{\mu}$. The pairwise interactions between particles, described by exchange constants J_{ij} , thus also have potential energy:

$$U = -J_{ij}\vec{\mu}_1 \cdot \vec{\mu}_2$$

We will ignore the short-range Pauli exclusion interactions.

Now, consider a collection of particles $\vec{\mu}_i$ in the presence of an external magnetic field \vec{B} . The Hamiltonian, which specifies the total energy of the system, is defined by the sum of all pairwise and all magnetic field energies:

$$E = -\frac{1}{2} \sum_i \sum_j J_{ij} \vec{\mu}_i \cdot \vec{\mu}_j - \sum_i \vec{\mu}_i \cdot \vec{B} \quad (1)$$

In most cases, working with this Hamiltonian is intractable. Luckily, we can simplify it by making several strategic assumptions.

First, we assume all atoms are fermionic spin- $\frac{1}{2}$ and identical. Then the magnetic moments simplify to $\vec{\mu}_i = \mu\sigma_i$, where $\sigma_i \in \{-1, 1\}$ is the spin of the atom.

Second, we make a mean-field approximation and assume that the atoms are arranged in a regular lattice, and that the strength of pairwise interactions are negligible for non-adjacent pairs.

Coalescing constants, the Hamiltonian reduces to:

$$E = -J \sum_i \sum_{j \in \text{adj}(i)} \sigma_i \sigma_j - \sum_i \sigma_i B_i \quad (2)$$

Following the Boltzmann distribution, the probability of some state $\vec{\sigma}$ at inverse temperature β is:

$$P(\vec{\sigma}) = \frac{1}{Z} e^{-\beta E(\vec{\sigma})} \quad (3)$$

2 Sample Based Methods of Inference

Say we want to test if a transition is favored or not. In the Ising model, a transition is defined by a change in one or more spins.

Say we flip one spin σ_i in $\vec{\sigma}$ to transition to state $\vec{\sigma}'$. We can measure whether this transition will be favored or not using the Boltzmann distribution. Namely, if $P(\vec{\sigma}') > P(\vec{\sigma})$ then the transition is favored. Alternatively, we could compute the ratio of probabilities. It turns out that for the Ising model this ratio has a nice form:

$$\frac{P(\vec{\sigma}')}{P(\vec{\sigma})} = \frac{e^{-\beta E(\vec{\sigma}')}}{e^{-\beta E(\vec{\sigma})}} = e^{-\beta \Delta E} \quad (4)$$

References