Lecture 1 - Introduction

We consider a random variable $x_i \in \mathcal{X}$ where $\mathcal{X}$ is a **state space**.

Given degrees of freedom $i = 1, \dots, N$ we can define different configurations in a configuration space

$$x \in \bigtimes_N \mathcal{X} = \mathcal{X}^N$$

We can, thus, define a distribution over configurations, defined by Boltzmann's equation:

$$P(x) = \frac{1}{Z} e^{-\beta E(x)}$$

where $\beta = \frac{1}{T}$ is the **inverse temperature**.
$Z = \sum_x e^{-\beta E(x)}$ is the **partition function**.

For instance, consider an Ising spin

$$s_i \in \{\pm 1\}$$

with energy function $E(s_i) = -h s_i$, where h is a constant for the **magnetic field**.
Then,

$$Z = e^{\beta h} + e^{-\beta h}$$

and the Boltzmann equation is

$$P(\ldots) \quad e^{-h\beta s_i}$$

$$P(s_i) = \frac{\quad}{e^{\beta h} + e^{-\beta h}}$$

Now what if we have an entire configurations of Ising spins with N degrees of freedom?
Suppose spins are independent, then

$$E(s) = -h \sum_i s_i$$

so the Boltzmann Equation is

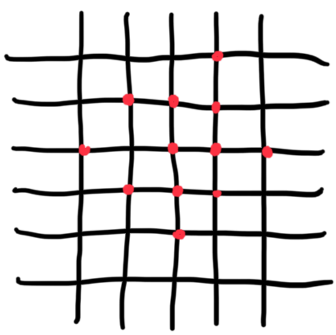
$$P(s) = \frac{1}{Z} e^{\beta h \sum_i s_i} = \frac{1}{Z} \prod_i e^{\beta h s_i}$$

where Z is a partition function over all the possible configurations.

Examples

① Ising Spins

Consider $s_i \in \{\pm 1\}$ with configuration $s \in S^N$



$E(s) = -J \sum s_i s_j - h \sum s_i$ implying neighbouring interactions between spins.

The Boltzmann equation is

$$P(s) = \frac{1}{Z} e^{-\beta E(s)}$$

we see how low energy configurations are favoured. Indeed, energy is minimized when neighbouring spins point in the same direction. This increases probability mass on such configurations.

We are interested on the mean magnetization. We define the magnetization as the expected value of an Ising spin

$$\langle s_i \rangle$$

we can compute this.

$$\langle s_i \rangle = \sum_i P(s_i) s_i = \frac{e^{\beta h}}{e^{\beta h} + e^{-\beta h}} - \frac{e^{-\beta h}}{e^{\beta h} + e^{-\beta h}}$$

$$= \tanh(\beta h)$$

We see that given a certain magnetic field h, the magnetization changes with Temperature. When $\beta \to \infty$ so $T \to 0$, then $\langle s_i \rangle = 1$, the maximum possible.

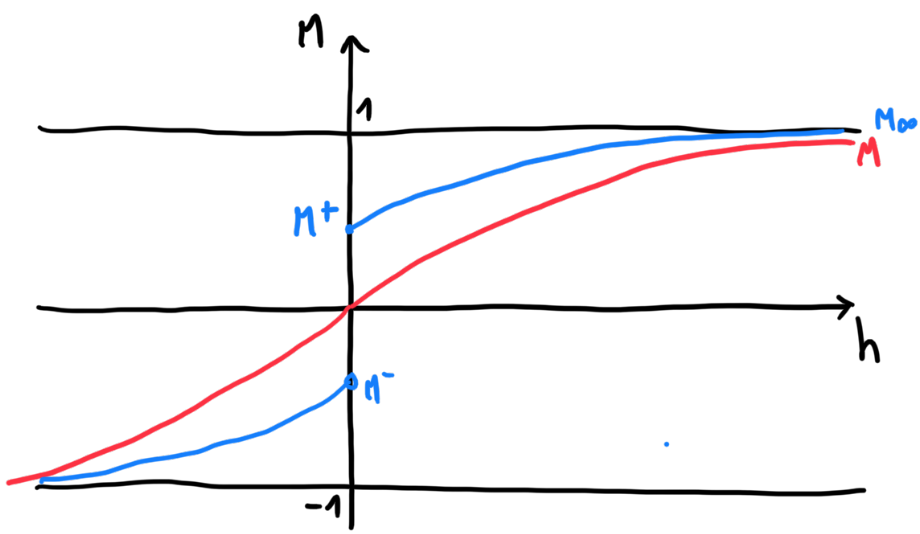
However, when $\beta \to 0^+$, so $T \to \infty$, then $\langle S_i \rangle \to 0$.
The same goes if we fix β and let h change. When $h \to \infty$, $\langle S_i \rangle = 1$, while when $h \to 0^+$, then $\langle S_i \rangle \to 0$.

Given a configuration S with N degrees of freedom, we are interested in the mean magnetization

$$M = \frac{1}{N} \sum_i \langle S_i \rangle$$

and in particular, we want to understand M as $N \to \infty$.
We plot M and M_∞ as functions of h, where

$$M_\infty = \lim_{N \to \infty} M$$



- For N finite, when $h=0$,

$$M = \frac{\cancel{N} \tanh(0)}{\cancel{N}} = 0$$

for $h \to \infty$, $M=1$ and for $h \to -\infty$, $M=-1$.

- For $N \to \infty$, when $h \to 0^+$, there is a spontaneous mean magnetization, as opposed to when N is finite. Therefore, the structure of a magnet tends to remain stable also once we exit a magnetic field. However, this breaks down once we let Temperature change. Out of a magnetic field, when $T \to \infty$, mean magnetization goes to 0, while M_+ is 1 when $T \to 0$. We thus have a so called phase transition. M_+ is positive until a critical temperature T_c is reached. Once this is surpassed, $M_+ = 0$.

Scaling Thermodynamic Limit

Given configurations $x \in X^N$ we can express energy as

$$E(x) = N \cdot \mathcal{E}(x)$$

This allows us to express the partition function in an easier way.
We know that

$$Z = \sum e^{-\beta E(x)}$$

x -

We can compute the number of configurations displaying average energy per particle

$$\mathcal{E}(x) = \mathcal{E} = \frac{E(x)}{N}$$

Suppose this particular configuration has Nf spins facing the opposite direction, then we have a total of

$$\binom{N}{Nf}$$

such configurations.

Thus we can write the partition function as

$$Z = \sum_{\mathcal{E}} e^{N\Delta(\mathcal{E}) - \beta N \mathcal{E}}$$

where $N\Delta(\mathcal{E})$ is the number of configurations with energy per spin level $\mathcal{E}$.

We immediately see that when $N \to \infty$ and becomes very large, there is one configuration that starts dominating, hence a particular energy level $\mathcal{E}^*$; we say that

$$\mathcal{E} \sim \mathcal{E}^*$$

This greately simplifies the model because the energy distribution becomes very peaked around one single configuration instead of many. Here fluctuations are minimal, therefore the system is balanced.
Of course this assumes a fixed β. If we let β change, then:

- If $\beta \to 0$, $T \to \infty$, then all the configurations become equally likely and energetic fluctuations can swing wildly, thus ending up with a chaotic system
- If $\beta \to \infty$, $T \to 0$, distribution is concentrated around ground configurations, fluctuations are minimal.

This implies a phase transition after T_c.

We now define the free energy density:

$$f = \frac{F}{N} = -\frac{1}{\beta N} \log Z$$

where F is the free energy:

$$F = -\frac{1}{\beta} \log Z$$

The entropy is:

$$S = -\sum_x P(x) \log P(x)$$

$$= -\sum_x P(x) \left[-\beta E(x) - \log Z \right]$$

$$= -\sum_x -\beta P(x) E(x) - P(x) \log Z$$

This is Shannon's Entropy, measuring the average unpredictability of a system.
The higher the number of potential configurations, the higher the entropy value.

We introduce the Internal energy:

$$U = -\frac{\partial \log Z}{\partial \beta} = \langle E(x) \rangle$$

Thus, rewriting the entropy as

$$S = \beta U + \log Z = \beta U - \beta F$$

and

$$F = U - \frac{1}{\beta} S$$

This means that when we understand $\log Z$, then we can obtain U, F and S of the system.
Z is fundamental because as a partition function, it gives information about the energetic spectrum, or how energy is distributed among the different configurations of the system.