15.1 Ising Model

The studied instance is $\sqrt{n} \times \sqrt{n}$ box of two-dimensional grid $\mathbb{Z}^2$. For each site of the lattice, it only takes $+1$ or $-1$. So the configuration is $\sigma : V \to \{+1, -1\}$ and $\Omega = \{+1, -1\}^V$.

For $\sigma \in \Omega$, energy is calculated by using the Hamiltonian

$$H(\sigma) = -\sum_{(i,j) \in E} (\sigma_i, \sigma_j) = -(\#\text{monoedges} - \#\text{antiedges})$$  \hspace{1cm} (15.1)

Boltzmann or Gibbs Distribution is

$$\mu(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z}$$  \hspace{1cm} (15.2)

where $Z = \sum_{\sigma \in \Omega} e^{-\beta H(\sigma)}$ is a partition function and $\beta = \frac{1}{KT}$ is inverse temperature ($\beta > 0$). This is the ferromagnetic Ising model, for antiferromagnetic, it has $\beta < 0$.

So most likely configurations are all $+$ or all $-$. But there are a lot more configurations with half $+$ and half $-$. In these cases, energy or entropy, which domains? It depends on $\beta$.

i) $\beta = 0$ (temperature is infinite): every configuration is equally likely so $\mu$ is dominated by balanced configurations (half $+$ and half $-$), which has min energy and max entropy.

ii) $\beta = \infty$ (temperature is zero): all $+$ and all $-$ are the only two configurations with positive probability, which has max energy and min entropy.

iii) Then we discuss the case when $0 < \beta < \infty$
Figure 15.2: Boundary condition example

For $\sqrt{n} \times \sqrt{n}$ box, $\partial V$ are the vertices on the internal boundary of $V$. Boundary condition is assigned $\tau : \partial V \rightarrow \{+1, -1\}$. Then $\Omega_\tau = \{\sigma \in \Omega : \sigma(\partial V) = \tau(\partial V)\}$ = configurations on $V$ which are consistent with $\tau$ on $\partial V$.

For $\sigma \in \Omega_\tau$

$$\mu_\tau(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z_\tau}$$  \hspace{1cm} (15.3)

where $Z_\tau = \sum_{\sigma \in \Omega_\tau} (e^{-\beta H(\sigma)})$

Let $O = \text{origin}$ be the center of $(2l + 1) \times (2l + 1)$ box, $l = \Theta(\sqrt{n})$. Let

$$P_\tau^l = P_\tau(\mu_\tau(\sigma(O) = +)) = P_\tau(\text{origin is + for boundary condition } \tau)$$ \hspace{1cm} (15.4)

$P_\tau^l$ is maximized for $\tau = \text{all+}$, denote as $P_+^l$ and is minimized for $\tau = \text{all-}$, denote as $P_-^l$

When $l$ is finite, it’s clearly that $P_+^l \neq P_-^l$, and actually $P_+^l > \frac{1}{2} > P_-^l$.

What about for $l \to \infty$?

Is $\lim_{l \to \infty} P_+^l \overset{?}{=} \lim_{l \to \infty} P_-^l$?

### 15.1.1 Phase Transition

$$\exists \beta_c,$$

$\forall \leq \beta_c$, $P_+^l = P_-^l (\text{disordered})$

$\forall > \beta_c$, $P_+^l \neq P_-^l (\text{long-range order})$

where,

$$\beta_c(q) = \frac{q - 1}{q} \log(1 + \sqrt{q})$$ \hspace{1cm} (15.5)

when $q = 2$, it’s Ising model

when $q > 2$, $\Omega = 1, 2, ..., Q^V$, it’s Potts Model

what about when $\beta = \beta_c$? It actually depends on $q$ as the figures 15.3 and 15.4.

For detail, please refer Onsager[1] ($q = 2$) and Beffara, Duminil-Copin '12[2] ($q > 2$)
15.1.2 Glauber Dynamics/ Gibbs Sampler

The goal is to sample from distribution $\mu$ to get Markov chain.

Transitions are made as follows:

From $X_t \in \Omega$ (no boundary condition)

1. Choose $\nu \in V$ v.a.r.
2. For all $\omega \neq \nu$, set $X_{t+1}(\omega) = X_t(\omega)$.
3. Choose $X_{t+1}(\nu) = \mu(\sigma(\nu)|\sigma(\omega) = X_{t+1}(\omega)$ for all $\omega \neq \nu$)

In other words,

$$X_{t+1}(\nu) = \begin{cases} + \frac{e^{\beta(p-n)}}{1 - e^{\beta(p-n)} + e^{\beta(p-n)}} & \text{if } \nu \in \{+\} \\ - \frac{e^{\beta(n-p)}}{1 + e^{\beta(n-p)} + e^{\beta(p-n)}} & \text{if } \nu \in \{-\} \end{cases}$$

where $p$ is number of + neighbors and $n$ is number of - neighbors.

$\forall \beta < \beta_c$: $T_{mix} = (n \log n)$

$\forall \beta > \beta_c$: $T_{mix} = e^{\Omega(\sqrt{n})}$

For $q \leq 3$, when $\beta = \beta_c$: $T_{mix} = p\log(n)$

For $q \geq 5$, when $\beta = \beta_c$: $T_{mix} = e^{\Omega(\sqrt{n})}$

How might we get around "torpid" mixing for $\beta > \beta_c$?

There are two approaches: Simulated annealing and Metropolis-coupled Markov Chain Monte Carlo.

15.1.3 Simulated Annealing

Idea: physical annealing is the process that heat a material above recrystallization and then slowly cooling. To get the desired $\beta$, start from $\beta_0 = 0$ and the sequence of inverse temperatures is $\beta_0 < \beta_1 < ... < \beta_N = \beta$.
For $i = 0 \to N$, repeat the following procedure:

1. Run Glauber dynamics for a large number of steps $T$ at $\beta_i$.
2. Let $X^i_T$ be the final step.
3. Let $X^{i+1}_o = X^i_T$ be the initial step for $\beta^{i+1}_i$.

Naive cooling schedule: $\beta^{i+1}_i = \beta_i (1 + \frac{1}{n})$

15.1.4 Metropolis-coupled Markov Chain Monte Carlo

$MC^3$ runs $N$ chains simultaneously, which contains one cold chain (the one that samples) and several heated chains. For the $i$th chain, it runs at $\beta_i$ temperature.

At step $t$, configuration is $(x^0_t, x^1_t, ..., x^N_t)$

i) With probability $\frac{1}{2}$:
   all $N+1$ chains do Glauber move (or choose $i \in \{0, 1, ..., N\}$ v.a.r, do a Glauber step for $X^i_t$, others stay the same)

ii) With probability $\frac{1}{2}$:

1. choose $i \in \{0, 1, ..., N\}$.
2. $X' = (x^0_t, ..., x^{i-1}_t, x^{i+1}_t, x^i_t, x^{i+2}_t, ..., x^N_t)$, which swap states $i$ and $i+1$.
3. Set $X_{t+1} = X'$ with probability $\min \{1, \frac{\omega_{\beta_i}(X_t(i+1))\omega_{\beta^{i+1}_i}(X_t(i))}{\omega_{\beta_i}(X_t(i))\omega_{\beta^{i+1}_i}(X_t(i+1))}\}$

References
