Lecture 15: October 17

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15.1 Ising Model

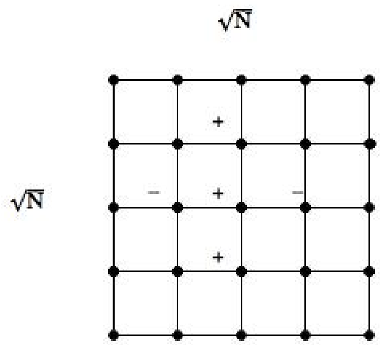

Figure 15.1: Ising model example

The studied instance is $\sqrt{n} * \sqrt{n}$ 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

$$H(\sigma) = -\sum\nolimits_{(i,j)\in E}(\sigma_i, \sigma_j) = -(\#monoedges - \#antiedges) \tag{15.1}$$

Boltzmann or Gibbs Distribution is

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

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 ferromagentic Ising model, for antiferromagentic, it has $\beta < 0$.

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

i) $\beta = 0$ (temperature is infinite): every configuration is equally likely so μ 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 $0 < \beta < \infty$

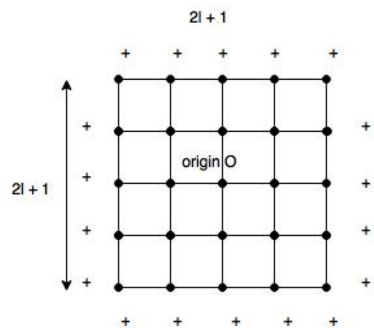

Figure 15.2: Boundary condition example

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

For $\sigma \in \Omega_\tau$

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

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

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

$$P^l_\tau = P_r(\mu_\tau(\sigma(O) = +)) = P_r(origin\ is\ +\ for\ boundary\ condition\ \tau) \tag{15.4}$$

P^l_τ is maximized for $\tau = all+$, denote as P^l_+ and is minimized for $\tau = all-$, 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 $\lim_{l\to\infty} P^l_+ \stackrel{?}{=} \lim_{l\to\infty} P^l_-$

15.1.1 Phase Transition

$\exists \beta_c$,

$\quad \forall \leqslant \beta_c,\ P^l_+ = P^l_-(disordered)$

$\quad \forall > \beta_c,\ P^l_+ \neq P^l_-(long-range\ order)$

where,

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

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)

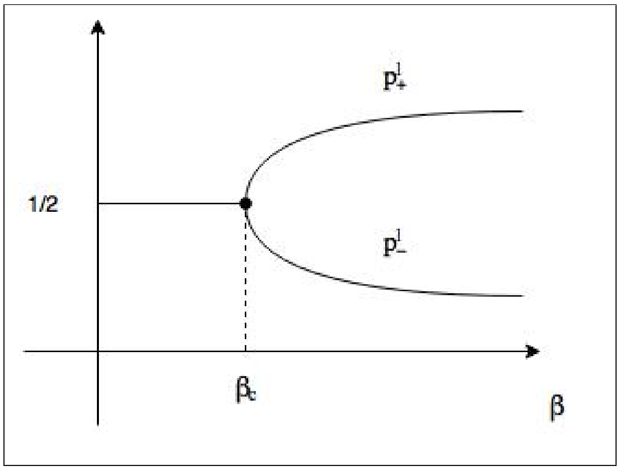

Figure 15.3: 2nd order phase transition for q $\leqslant$ 4

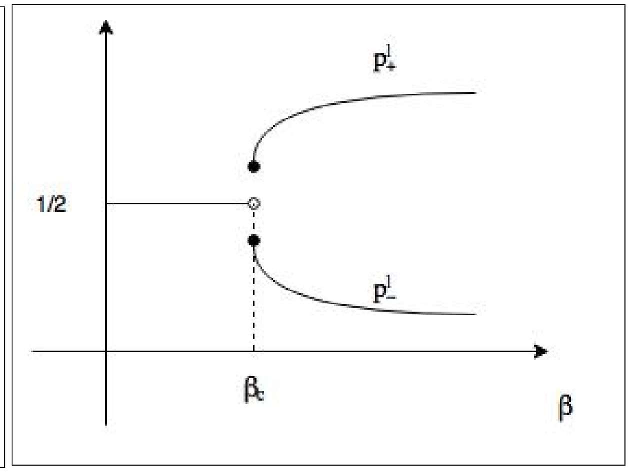

Figure 15.4: 1st order phase transition for q $>$ 4

15.1.2 Glauber Dynamics/ Gibbs Sampler

The goal is to sample from distribution μ 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,

$$X_{t+1}(\nu) = \begin{cases} + & \frac{e^{\beta(p-n)}}{e^{\beta(p-n)}+e^{\beta(p-n)}} \\ - & 1 - \frac{e^{\beta(p-n)}}{e^{\beta(p-n)}+e^{\beta(p-n)}} \end{cases} = \begin{cases} + & \frac{1}{1+e^{2\beta(n-p)}} \\ - & \frac{e^{2\beta(n-p)}}{1+e^{2\beta(n-p)}} \end{cases} \tag{15.6}$$

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

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

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

For $q \leqslant 3$, when $\beta = \beta_c$: $T_{mix} = ploy(n)$

For $q \geqslant 5$, 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 β, start from $\beta_0 = 0$ and the sequence of inverse temperatures is $\beta_0 < \beta_1 < ... < \beta_N = \beta$

For i = 0 $\rightarrow$ N, repeat the following procedure:

1. Run Glauber dynamics for a large number of steps T at β_i.
2. Let X_T^i be the final step.
3. Let $X_o^{i+1} = X_T^i$ be the initial step for β_{i+1}

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

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 ith chain, it runs at β_i temperature.

At step t, configuration is $(x_t^0, x_t^1, ..., x_t^N)$

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_t^i, others stay the same)

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

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

References

[1] Onsager, Lars, "Crystal statistics. I. A two-dimensional model with an order-disorder transition" *Physical Review* **65.3-4** (1994), 117.

[2] Beffara, Vincent, and Hugo Duminil-Copin, "The self-dual point of the two-dimensional random-cluster model is critical for q 1" *Probability Theory and Related Fields* **153.3** (2012), 511-542.