Mathematics 9th #4.
'23.9.10.
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Concepts in Stochastic Models & Processes

I. Stochastic model & process.

- Why is it important?
  - Statistical mechanics :
    If we solve it deterministically, then we have to work w/ system of N mols of equations.

    ⇝ let them behave randomly, and study their macroscopic behavior!
  - Ising model, percolation, random graph, Brownian motion, ...

- Preliminary : Probability theory.
  - Probability space : $(\Omega, \mathcal{F}, \mathbb{P})$.
    - Ω : space of states.
    - $\mathcal{F}$: σ-algebra.
    - $\mathbb{P}$: probability measure $(\mathbb{P}[\Omega] = 1)$.
  - $A \in \mathcal{F}$: event.
  - X : $\mathcal{F}$-measurable function on Ω : random variable.
  - $\mathbb{E}[X] := \int_\Omega X \, d\mathbb{P}$: expectation.

II. Phase transition.

- When we have a family of models, parametrized by a variable, we often can observe a "phase transition" phenomenon.

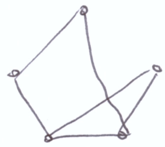
subcritical regime — supercritical regime. → parameter p.

$\begin{pmatrix} \cdot \text{ almost surely} \\ \cdot \text{ with high probability} \\ \cdot \text{ etc...} \end{pmatrix}$ A critical point $p = p_c$ $\begin{pmatrix} \cdot \text{ almost surely} \\ \cdot \text{ with high probability} \\ \cdot \text{ etc...} \end{pmatrix}$ B.

- e.g. 1. Erdös - Renyi graph.

· Erdös - Renyi graph $G_{n,p} \subseteq K_n$ $(p \in [0,1])$.

: $\mathbb{P}_p[G_{n,p} = G] = p^{\#\text{ edges in } G} \cdot (1-p)^{\binom{n}{2} - \#\text{edges in } G}$.



· Q. Given a graph H, what is the probability that $H \subseteq G_{n,p}$?

· $H = \Delta$: let $T = \#$ of Δ in $G_{n,p}$.

$$\mathbb{E}T = \binom{n}{3} \cdot p^3 \longrightarrow \begin{cases} 0 & \text{if } p \ll \frac{1}{n} \\ \infty & \text{if } p \gg \frac{1}{n} \end{cases}.$$

$$\mathbb{E}T^2 = \sum_{\Delta} \mathbb{E}\Delta^2 + \sum_{\Delta_i \neq \Delta_j} \mathbb{E}\Delta_i\Delta_j = \binom{n}{3} \cdot p^3 + 3\binom{n}{3}(n-3) \cdot p^5 + \left[\binom{n}{3}\binom{n-3}{3} + 3\binom{n}{3}\binom{n-3}{2}\right] \cdot p^6$$

(Second moment method) $\mathbb{P}[T=0] \leq \mathbb{P}[|T - \mathbb{E}T| \geq \mathbb{E}T] \overset{\text{chebyshev}}{\leq} \frac{\operatorname{Var} T}{(\mathbb{E}T)^2} \to 0$ if $p \gg$

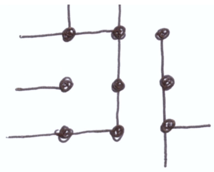
$$\Rightarrow \mathbb{P}[H \subseteq G_{n,p}] \longrightarrow \begin{cases} 0 & \text{if } p \ll \frac{1}{n} \\ 1 & \text{if } p \gg \frac{1}{n} \end{cases}.$$

· (Erdös - Renyi, Bollobás) $\forall H$, $m_H := \min\left\{ \frac{v_K}{e_K} : K \subseteq H \right\}$.

$$\mathbb{P}[H \subseteq G_{n,p}] \longrightarrow \begin{cases} 0 & \text{if } p \ll n^{-m_H} \\ 1 & \text{if } p \gg n^{-m_H} \end{cases}.$$

$\nexists H$ w.h.p. — $\exists H$ w.h.p.

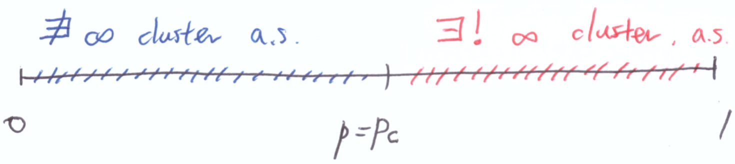
0 — $p \asymp n^{-m_H}$ — 1



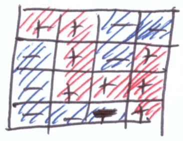
- e.g. 2. Percolation.

  - d-dim'l hypercubic lattice $\mathbb{L}^d = (\mathbb{Z}^d, \mathbb{E}^d)$, $p \in [0,1]$.
  - Percolation : $\omega \in \Omega = \{0,1\}^{\mathbb{E}^d}$. $\omega(e) \sim Ber(p)$ i.i.d. $\forall e \in \mathbb{E}^d$.
  - Q. What is the probability that we have an infinite cluster?
  - $\theta(p) := \mathbb{P}_p[\,0 \text{ is in an } \infty \text{ cluster}\,]$.

    $p_c := \sup\{p : \theta(p) = 0\}$.
  - FACT)



(∵ ∄, ∃ : Use 0-1 law.
∃! : Pretty complicated... Read [Grimmett '99 - Percolation].)



- e.g. 3. 2-dim'l Ising model.

- $\Lambda = [0, L]^2 \subseteq \mathbb{Z}^2$ box, $\sigma \in \{+1, -1\}^{\Lambda} = \Omega$.

- Hamiltonian: $H(\sigma) = -\underset{J>0 \text{ interaction strength}}{J} \cdot \sum_{x \sim y} \mathbb{1}\{\sigma_x = \sigma_y\} - \underset{\text{external magnetic field}}{h} \sum_{x} \mathbb{1}\{\sigma_x = +1\}$.

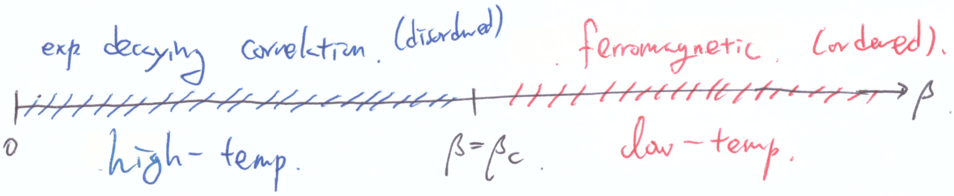
- $\mathbb{P}_\beta[\sigma] = \frac{1}{Z_\beta} e^{-\beta H(\sigma)}$ "Gibbs measure" inverse temperature $\beta = \frac{1}{k_B \cdot T} > 0$.

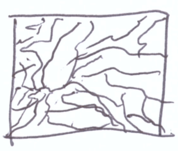
- let $h = 0$. (zero magnetic field), $J = 1$.
  Passing to weak limit as $L \to \infty$,
  we can define an Ising model on $\mathbb{Z}^2$.

- Q. For two sites $x, y \in \mathbb{Z}^2$, how are σ_x, σ_y correlated?

- FACT) For $\beta_c = \log(1+\sqrt{2})$,

$$\mathbb{P}_\beta[\sigma_x = \sigma_y] - \frac{1}{2} \xrightarrow{|x-y| \to \infty} \begin{cases} 0 \ \text{exponentially fast,} & \text{if } \beta < \beta_c \\ c(\beta) > 0 & \text{if } \beta > \beta_c. \end{cases}$$





III. Glauber dynamics & mixing time

- Random process.

  ÷ Basically, it is a collection of random variables (X_t), where $t \in \mathbb{Z}_{\geq 0}$ or $\mathbb{R}_{\geq 0}$.

  - It is called a Markov chain if it is "memoryless",

    i.e., the conditional distribution of future states depends only upon the present state:

    $$\mathbb{P}[X_t \in A \mid \mathcal{F}_s] = \mathbb{P}[X_t \in A \mid X_s] \quad \forall A \in \mathcal{F}, \ s<t.$$

- Markov Chain Monte Carlo algorithm.

  - Q. Given a stochastic model, how can we sample (simulate) it?

  - Idea: Markov Chain Monte Carlo (MCMC).

    Construct a Markov chain on the state space

    whose stationary measure is the probability measure we want.

    Classical FACT) If an ergodic Markov chain X_t has stationary measure $\mathbb{P}$,

    then $\mathbb{P}^t_{X_0} \xrightarrow{t\to\infty} \mathbb{P} \quad \forall X_0 \in \Omega$.

  ※ Total variation distance

  $$\|\mathbb{P}_1 - \mathbb{P}_2\|_{TV} := \sup_{A\in\mathcal{F}} |\mathbb{P}_1[A] - \mathbb{P}_2[A]| . \quad (\in [0,1]).$$

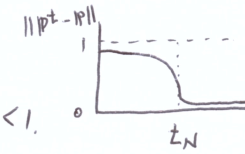
- Mixing time.

  $$t_{mix}(\varepsilon) := \inf\left\{ t : \max_{X_0\in\Omega} \|\mathbb{P}^t_{X_0} - \mathbb{P}\|_{TV} \leq \varepsilon \right\}. \qquad 0<\varepsilon<1.$$

  Conventionally, write $t_{mix} = t_{mix}(\frac{1}{4})$. (We may pick any $\varepsilon < \frac{1}{2}$).

- Cutoff:

  : A family of process exhibits cutoff if $\displaystyle\lim_{N\to\infty} \frac{t_{mix}(\varepsilon)}{t_{mix}(1-\varepsilon)} = 1 \quad \forall_{0<\varepsilon<1}$.



- Glauber dynamics.

  - Return to the finite-volume Ising model on $\Lambda = [0, L]^2$.

  - Equip $\Omega = \{\pm 1\}^{\Lambda}$ w/ a set of undirected edges E

    : $\sigma \sim \sigma'$ if $\sigma_x \neq \sigma'_x$ exactly at one site.

  - Glauber dynamics (σ_t) on Ω :

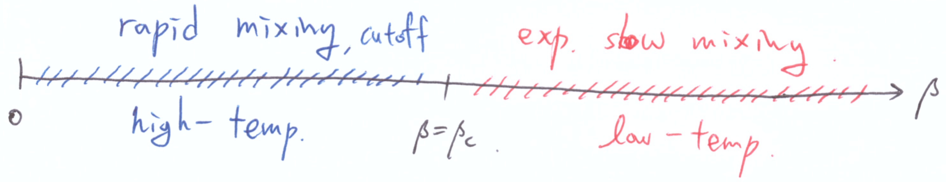
    : continuous time Markov process w/ transition rates "single spin flip"

$$c_\beta(\sigma, \sigma') = \begin{cases} e^{-\beta[H(\sigma') - H(\sigma)]_+} & \text{if } \sigma \sim \sigma' \\ 0 & \text{otw.} \end{cases}$$

  $\rightsquigarrow$ We have stationary measure $\mathbb{P}$, that is reversible & ergodic.

- FACT) $\cdot$ $\beta < \beta_c$: $t_{mix} = O(L^2 \log L)$: "coupon-collecting time" & cut-off.

  $\cdot$ $\beta > \beta_c$: $t_{mix} \geq e^{c(\beta) \cdot L}$ $\exists\, c(\beta) > 0$. [Lubetzky - Sly '14].



$\hookrightarrow$ This is a pretty universal picture!

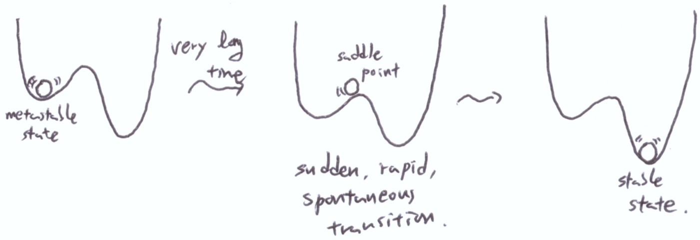
IV. Metastability.

- **Metastability**

  ≒ "Spontaneous transition from a 'fake' stable state to the stable state"

  - e.g. • supercooled water

    • diffusion w/ gradient drift



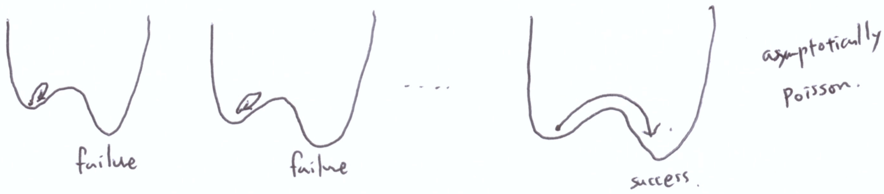
  - Common indicators.

    · exponential hitting time : $\tau_n = \inf\{t : X_t^n \in s\}$.

$$\Rightarrow \frac{\log \mathbb{E}_{im}\tau_n}{n} \xrightarrow{n\to\infty} \exists\, c > 0.$$

(cf. large deviations, Friedlin-Wentzell theory.)

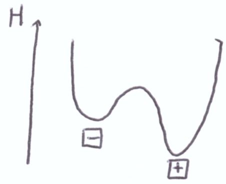
    · "independent" attempts : $\dfrac{\tau_n}{\mathbb{E}\,\tau_n} \xrightarrow{n\to\infty} \mathrm{Exp}(1)$ in distribution.



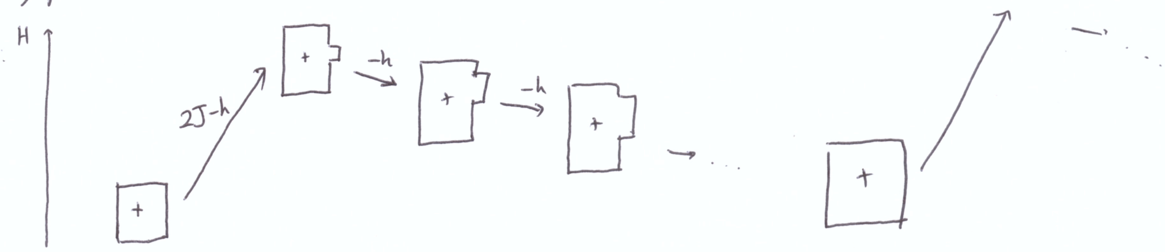
- Metastability of Glauber dynamics.

  - Now we consider $\Lambda = [0, L]^2$ torus, $J > 0$, $h \in (0, 2J)$.

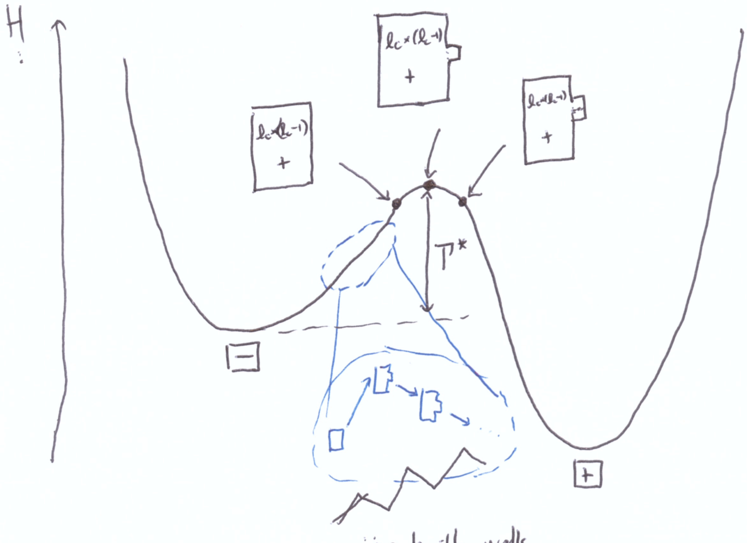
  - metastable state $\boxed{-}$: $\sigma_x = -1 \ \forall x$.
    stable state $\boxed{+}$: $\sigma_x = +1 \ \forall x$.



  - typical (most-likely) path $\boxed{-} \longrightarrow \boxed{+}$.



  - critical droplet size $\ell_c = \left\lceil \frac{2J}{h} \right\rceil$.



FACT) $\mathbb{E}\,\tau_{\boxminus \to \boxplus} \sim K e^{\beta \Gamma^*}$ where $\Gamma^* = J \cdot (4\ell_c) - h \cdot (\ell_c(\ell_c - 1) + 1)$.

$$K = \frac{3}{4(2\ell_c - 1)} \frac{1}{|\Lambda|}.$$

(See [Bovier-Hollander '15 - Metastability].)