Markov Chain
and
Markov Process

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What is a Markov Chain and Markov Process

- A stochastic process describing a sequence of possible events with the **Markov property** (memoryless).
- Discrete vs. Continuous
  - Discrete-time Markov chain (DTMC) ⇒ Markov Chain
  - Continuous-time Markov chain (CTMC) ⇒ Markov Process
- The countable set $\mathbb{S}$ consisting of the possible states of S_i is called the *state space* of the chain.

Discrete-time Markov chain

- If we use $\mathrm{S}_t \in \mathbb{S}$ to represent the system state at time t.
- Then for all $s_0, s_1, \ldots, s_t, s_{t+1}$
- The probability of system state at time $t+1$ is

$$P(S_{t+1} = s_{t+1} \mid S_t = s_t, S_{t-1} = s_{t-1}, \ldots, S_0 = s_0)$$

$$= P(S_{t+1} = s_{t+1} \mid S_t = s_t)$$

Continuous-time Markov chain

- If we use $S(t) \in \mathbb{s}$ to represent the system state at time t.
- The current time is n.
- Then the system state of next moment is $S(t)$.
- For $\dots p_3 < p_2 < p_1 < n < t$
- The probability of system state of next moment is

$$P(\,S(t) = s(t) \mid S(n) = s(n), S(p_1) = s(p_1), S(p_2) = s(p_2), \dots\,)$$
$$= P(\,S(t) = s(t) \mid S(n) = s(n)\,)$$

Representation

- For a finite state space
- Define the state basis is a row vector
- If we define $p_{ij} = P(\, S_{n+1} = i \mid S_n = j\,)$
- Then we can define one-step transition (probability) matrix

$$\mathbf{P} \equiv \begin{bmatrix} p_{11} & p_{12} & p_{13} & \cdots & p_{1N} \\ p_{21} & p_{22} & p_{23} & \cdots & p_{2N} \\ p_{31} & p_{32} & p_{33} & \cdots & p_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ p_{N1} & p_{N2} & p_{N3} & \cdots & p_{NN} \end{bmatrix}$$

Example - Monopoly game

Properties

- Irreducibility
  - We can go to any state j from any state i
  - For any 2 state i, j, $\exists$ step t so that $\mathbf{P}_{ij}^{t} > 0$, we call the Markov chain is irreducibility.
- Periodicity
  - From a state i , after starting, how many steps does it take to return to this state, and whether these steps have a common "cycle"
  - If a Markov chain is periodicity, then we can find

$$d(i) = gcd\{t \geq 1 \mid P_{ii}^{t} > 0\} > 1$$

Properties

- Absorbing state
  - When Markov chain going into a state, it will not change to any other state, then we call the state absorbing state.

$$P_{ii} = 1, P_{ij} = 0 \text{ for } i \neq j$$

- Stationary distribution
  - When a stationary distribution π is a (row) vector, whose entries are non-negative and sum to 1, is unchanged by the operation of transition matrix **P** on it and so is defined by
  - $\sum \pi_i = 1$; $\pi\mathbf{P} = \pi$

Properties

- Expected return time
  - After starting from state i, how many steps are expected to be required to return to the state for the first time?
    $$m_i = E[T_i|S_0 = i]$$
  - $m_i = 1 + \sum_{i \neq j} \mathbf{P}_{ij} m_{ji}$, for m_{ji} is expected time from state j to i
  - $m_i < \infty$, state i is recurrent state
  - $m_i = \infty$, state i is transient state
  - For an irreducible, aperiodic, and finite state space Markov chain: $m_i = {}^{1}/_{\pi_i}$

Properties

- Ergodicity
  - A Markov chain is said to be ergodic if, regardless of the initial state, the system can reach all states after multiple transitions, and the distribution converges to a unique stationary distribution.
  - The Markov chain is said to be ergodic iff a system is irreducible, aperiodic and positive recurrence($m_i < \infty$ for any state i)
  - If the Markov chain is ergodicity, then there are some properties
    - Unique stationary distribution, π is unique
    - Convergence, $lim_{t\to\infty}\pi^{(0)}\mathbf{P}^t = \pi$

Example - Brownian motion

- The Brownian motion will follow the Wiener process, which is a Markov Process.
- Wiener process
  - $W(0) = 0$.
  - It has independent increment: for any $0 \leq s < t$, the increment $W(t) - W(s)$ is independent of the past $\{W(u), u \leq s\}$
  - The increments are normally distributed: $W(t) - W(s) \sim N(0, t - s)$.
  - Its sample paths are almost surely continuous.
  - 1Dim PDF: $f_{W_t}(x) = \frac{1}{\sqrt{2\pi t}} e^{-x^2/2}$

Example - Brownian motion

- Mapping to Markov Chain:
  - States → particle positions
  - Transitions → Probabilities of particle move to other positions.
  - Markov property → Next step depends only on the current position, not the past history.
- Application
  - Motion of suspended particles
  - Diffusion phenomena

Example - electron transfer

- What is Electron Transfer?
  - Electron transfer refers to the movement of an electron between distinct molecular or atomic sites, such as donor → acceptor.
- Mapping to Markov Chain:
  - States → Electron positions (donor, acceptor, bridge).
  - Transitions → Probabilities of electron jumping between positions.
  - Markov property → Next step depends only on the current position, not the past history.

Example - electron transfer

- Why Markov Chain?
  - Describes stochastic (random) hopping between discrete sites.
  - Captures both short-term dynamics and long-term (steady-state) distributions.
- Applications:
  - Electron transfer in biological systems (e.g., electron transport chain).
  - Charge transport in materials (e.g., semiconductors).
  - Redox reactions in chemistry.