Basics of Markov Chains

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Nov 2nd, 2021

Discrete Markov Chain

$\{X^{(n)} : n = 0, \dots, \}$ a sequence of dependent random variables, each $X^{(n)} \in S$ (state space).

We first discuss M.C in a discrete state space, say, $S = \{1, 2, \cdots, k\}$.

Definition: A Markov chain is a sequence of random variables $X^{(n)}$ such that

$$\begin{aligned} &P(X^{(n)} \in A_n | X^{(n-1)} \in A_{n-1}, \cdots, X^{(0)} \in A_0) \\ &= P(X^{(n)} \in A_n | X^{(n-1)} \in A_{n-1}) \end{aligned}$$

Let

$$p_{i,j}^{[n-1,n]} = P(X^{(n)} = j | X^{(n-1)} = i) \qquad \text{Transition Kernel}$$

We'll restrict ourselves to the time-invariant M.C.,that is, $p_{i,j}^{[n-1,n]}$ does not depend on the time reference point, but only depend on how far apart the two time points are. So $p_{i,j}^{[n,n+1]} = p_{i,j}^{[n-1,n]} = \cdots = p_{i,j}^{[0,1]}$ holds etc.

one-step transition kernel

- transition probability

$$p_{i,j} = p_{i,j}^{[1]} := P(X^{(n+1)} = j | X^{(n)} = i)$$

- Transition matrix

$$P := \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1k} \\ p_{21} & p_{22} & \cdots & p_{2k} \\ \vdots & \ddots & \cdots & \vdots \\ p_{k1} & p_{k2} & \cdots & p_{kk} \end{bmatrix}$$

$$p_{i,j} \geq 0, \ \forall i = 1, \cdots, k, \ \sum_{j=1}^{k} p_{i,j} = 1$$

m-step transition kernel

- transition probability

$$p_{i,j}^{[m]} := P(X^{(n+m)} = j | X^{(n)} = i)$$

- Transition matrix

$$P^{[m]} := \begin{bmatrix} p_{11}^{[m]} & p_{12}^{[m]} & \cdots & p_{1k}^{[m]} \\ p_{21}^{[m]} & p_{22}^{[m]} & \cdots & p_{2k}^{[m]} \\ \vdots & \ddots & \cdots & \vdots \\ p_{k1}^{[m]} & p_{k2}^{[m]} & \cdots & p_{kk}^{[m]} \end{bmatrix}$$

State distribution (occupation prob dist)

Time 0

$$\alpha^{(0)} = (\alpha_1^{(0)}, \cdots, \alpha_k^{(0)}), \text{where } P(X^{(0)} = i) = \alpha_i^{(0)}$$

Time 1

$$\alpha^{(1)} = (\alpha_1^{(1)}, \cdots, \alpha_k^{(1)}) = \alpha^{(0)} P$$

One can show that $\alpha^{(m)} = \alpha^{(0)} P^m$.

Proof

$$\begin{aligned} \alpha_j^{(1)} &= P(X^{(1)} = j) \\ &= \sum_{i=1}^{k} P(X^{(1)} = j, X^{(0)} = i) \\ &= \sum_{i=1}^{k} P(X^{(1)} = j | X^{(0)} = i) P(X^{(0)} = i) \\ &= \sum_{i=1}^{k} \alpha_i^{(0)} p_{i,j} \\ &= \alpha^{(0)} P \\ \alpha^{(2)} &= \alpha^{(1)} P = \alpha^{(0)} P^2 \\ &\vdots \\ \alpha^{(m)} &= \alpha^{(0)} P^m \end{aligned}$$

Also one can write $\alpha^{(m)} = \alpha^{(0)} P^{[m]}$.

Therefore,

$$P^{[m]} = P^m$$

Definition If a state distribution(π) satisfies:

$$\pi P = \pi$$

Then π is called a "steady state dist" (stationary distribution). note that it is the same as

$$\pi_j = \sum_{i=1}^{k} \pi_i p_{i,j}, \ \forall \ j = 1, 2, \cdots, k$$

The LHS π_j is steady state prob for the state j. The RHS $\sum_{i=1}^{k} \pi_i p_{i,j}$ is total probability flowing into state j from any states. To see the meaning of the steady state distribution, consider a scenario that at some step n, we reached the steady state distribution,

$$\alpha^{(n)} = \pi$$
$$\alpha^{(n+1)} = \alpha^{(n)}P = \pi$$

Therefore, once we reached the steady state distribution, the state distribution becomes stationary.

Find the steady state distribution: For a given P, note that

$$P^T \pi^T = 1\pi^T$$

So π^T is eigenvalue of P^T that corresponds to eigenvalue 1.

Markov Chain Monte Carlo methods(MCMC)

Most of the M.C. encountered in MCMC settings enjoy some nice properties. In particular, we're interested in M.C.s that satisfy the following three properties.

aperiodic

- A state i has period $v \in N$ if $p_{ii}^{[m]} > 0$ only holds for m that is a multiple of v
- A state is aperiodic if $p_{ii}^{[m]} > 0$ for all m sufficiently large, that is $v = 1$
- A chain is called "aperiodic" if all states are aperiodic

(positive) recurrent

- A state i is said to be recurrent, if when we run the M.C. from i continusously, we are guaranteed to return to i infinitely often and the first return happens within a finite numbers of steps on average
- A chain is called recurrent if all state are.

irreducible

The chain has a positive probability of eventually reaching any state, i.e.

$$\forall i, j \; p_{i,j}^{[n_0]} > 0 \; for \; some \; n_0$$

Summary

We restrict ourselves to "time inveriant" M.C. that are irreducible, aperiodic and (positive) recurrent. We call these M.C. "ergodic M.C.".

Theorem

Any ergodic M.C. has a steay state distribution π, i.e., $\pi P = \pi$, and

$$\pi_j = \lim_{n\to\infty} p_{i,j}^{[n]} \qquad \text{for all } i$$

that is, π is also the "long-run" distribution of the chain.

Example:

$$S = \{1, 2, 3\}$$

$$\alpha^{[0]} = (1, 0, 0)$$

$$P = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 \\ 1/5 & 0 & 4/5 \end{bmatrix}$$

$$\begin{aligned} P(X^{(1)}) &= \alpha^{[1]} \\ \alpha^{[1]} &= \alpha^{[0]}P = (1/2, 1/2, 0) \\ P(X^{(2)}) &= \alpha^{[2]} \\ \alpha^{[2]} &= \alpha^{[1]}P = (1/4, 1/2, 1/4) \\ &\vdots \\ \alpha^{[10]} &= \alpha^{[0]}P^{10} = (2/9, 2/9, 5/9) \end{aligned}$$

if n is large
$\alpha^{[n]}$ converges to (2/9, 2/9 , 5/9), is "long-run distribution".

Verify: $(2/9, 2/9, 5/9)P = (2/9, 2/9, 5/9)$

Sampling from steady-state distribution

Let $\alpha^{(m)}$ be the state distribution at time m. How can we obtain a sample from the steady-state distribution? One possibility is that we start N chains, let them run long enough, and collect those near-end-time values from all these chains. These values then become a sample from the steady-state distribution. With ergodicity, there is another possibility (more feasible), that is we collect a few of near-end-time values from a single M.C. that has run long enough, then this collection also can be seen as a sample from the steady-state distribution.

- single chain

$$\begin{gathered} X^{(1)} \sim \alpha^{(1)} \\ X^{(2)} \sim \alpha^{(2)} \\ \vdots \\ X^{(\infty)} \sim \alpha^{(\infty)} \equiv \pi \end{gathered}$$

- ensemble: the set of all possible chains

$$\begin{bmatrix} \text{chain 1} & \text{chain 2} & \cdots & \text{chain N} \\ X_1^{(1)} & X_2^{(1)} & \cdots & X_N^{(1)} \\ X_1^{(2)} & X_2^{(2)} & \cdots & X_N^{(2)} \\ \vdots & \vdots & \cdots & \vdots \\ X_1^{(\infty)} & X_2^{(\infty)} & \cdots & X_N^{(\infty)} \end{bmatrix}$$

The Law of Large Number

A ergodic M.C. has a very important property. That is, the time average of a simple realization approaches the average of all possible realization of their chains, **called ensemble**, at some particular point in the far future.

Goal: estimate $E(h(X^{(\infty)})) = \int h(x)\pi(x)dx$

The conventional law of large number says that, using the ensemble,

$$\frac{1}{N}\sum_{i=1}^{N} h(X_i^{(\infty)}) \to E(h(X^{(\infty)})) \text{ as } \ N \to \infty.$$

Ergodicity guarantees that, using just a single M.C.,

$$\frac{1}{T}\sum_{n=1}^{T} h(X^{(n)}) \to E[h(X^{(\infty)})] \text{ as } \ T \to \infty.$$

This provides the theoretical justification–why obtaining samples from a single M.C. after it has run long enough, we are effectively obtaining samples from the steady-state distribution.