Big Data Analysis (MA60306)

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Spring 2022-23, IIT Kharagpur

Lecture 24 March 30, 2023

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Random walks

Transition matrix A random process $\{X_0, X_1, \ldots\}$ with finite state space $S = \{s_1, s_2, \ldots, s_k\}$ is a (homogeneous) Markov chain with transition matrix $P = [p_{ij}] \in \mathbb{R}^{k \times k}$ if

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Example:

$$P = \begin{bmatrix} 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \end{bmatrix}$$

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Question Does the transition matrix have any special property?

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(i)
$$\pi_i \ge 0$$
 and $\sum_{i=1}^k \pi_i = 1$, and
(ii) $\pi P = \pi$, i.e. $\sum_{i=1}^k p_{ij} = \pi_j$, for $j = 1, ..., k$

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Question What is the meaning of this condition? Can we say that a Markov chain is stationary if and only if $p(X_{t+1} = y | X_t = x)$ is independent of t for any x, y?

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Question Is every Markov chain stationary? Can there exist more than one stationary distributions of a Markov chain?

reversible distribution A probability distribution π for a Markov chain on the state space $S = \{s_1, \ldots, s_k\}$ is called reversible for a Markov chain if for all $i, j \in \{1, \ldots, k\}$

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Observation If $\pi_i p_{ij}$ is interpreted as the amount of probability mass flowing at any time instant from the state s_i to s_j , then for reversible Markov chain, it is equal to the amount of probability mass flowing from s_j to s_i . (a sense of equilibrium/balance!)

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Homework For a reversible MC, if the initial distribution is stationary then $P(X_t = j | X_{t+1} = i) = p(X_{t+1} = j | X_t = i)$

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Observation For a reversible MC,

$$\sum_{j\in S} p_{ji}\pi(j) = \sum_{j\in S} p_{ij}\pi(i) = \pi(i)\sum_{j\in S} p_{ij} = \pi(i)$$

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Thus the period of s_i is the greatest common divisor of the set of times that the chain can return (i.e., has positive probability of returning) to s_i , given that we start with $X_0 = s_i$. If the period $s_i = 1$, then we say that the state s_i is aperiodic.

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A Markov chain is said to be aperiodic if all its states are aperiodic. Otherwise the chain is said to be periodic

Homework Consider the following Markov chain:

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Determine the periodicity, regularity and irreduciblity property of the Markov Chain.

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Existence and uniqueness Any irreducible and aperiodic Markov chain has exactly one stationary distribution.

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Example of a MC model Assume that a mosquito hops between the forehead, the left check and the right check of a person

There are three states

Suppose the rule is: At some time t, if the mosquito is sitting on the foreheaad then it will hop to left check at time t + 1

if it sits on the left check, it will stay there or move to the right check with probability 0.5 for each, and if it is on the right check then it will stay there or move to the forehead with probability 0.5 each.

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There are three states

Suppose the rule is: At some time t, if the mosquito is sitting on the foreheaad then it will hop to left check at time t + 1

if it sits on the left check, it will stay there or move to the right check with probability 0.5 for each, and if it is on the right check then it will stay there or move to the forehead with probability 0.5 each.

Then the transition matrix is

$$P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0.5 & 0.5 \\ 0.5 & 0 & 0.5 \end{bmatrix}$$

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Homework Determine the MC properties of the walk of the mosquito in the last example.

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GOAL How should we use the MC concept for simulating a pdf?

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GOAL How should we use the MC concept for simulating a pdf? MCMC was placed in the top 10 most important algorithms of the 20th century (SIAM news).

- \rightarrow Suppose $p(\mathbf{x})$ is the given pdf
- $\rightarrow\,$ Define a MC on a state space whose stationary distribution is the target density

A bit of history MCMC algorithm was discovered by physicists working on the atomic bomb at Los Alamos during World War II, and was first published in a chemistry journal. Metropolis et al. 1953.

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Math framework of MCMC algo To draw simulations from a target distribution π on a countable set S, define a stationary Markov chain or a transition matrix P which is irreducible and aperiodic such that the reversibility condition $p_{ij}\pi_i = p_{ji}\pi_j$ holds.

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Theorem (Justification of approximating the true average by sample average) Let X_n , $n \ge 0$ be an irreducible stationary Markov chain on a discrete state space S. Suppose X_n possess a stationary distribution π . If $\phi: S \to \mathbb{R}$ is such that $\mathbb{E}_{\pi}[\phi(X)]$ exists then for any initial distribution μ ,

$$\frac{1}{n}\sum_{k=1}^{n}\phi(X_k)\to^{\mathsf{a.s.}}\mathbb{E}_{\pi}[\phi(X)]$$

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Metropolis Algorithms

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Then the entries of the transition matrix are given by

$$egin{array}{rcl} p_{ij} &=& heta_{ij}\gamma_{ij}, \, i,j\in \mathcal{S}, \, j
eq i \ p_{ii} &=& 1-\sum_{j
eq i}p_{ij} \end{array}$$

where θ_{ij} is the probability that j is picked as a candidate state, and γ_{ij} is the probability of moving to the state j

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Transition matrix Choose the matrix or values θ_{ij} such that the transition matrix $P = [p_{ij}]$ is irreducible

Homework Is there a connection to accept-reject scheme here for choosing the candidate state?

Specific choices of θ_{ij}, γ_{ij} :

Independent Sampling: $\theta_{ij} = \pi(j)$ for all *i*, and $\gamma_{ij} \equiv 1$

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Homework Verifying the assumptions!