X_n ergodic Markov chain

$P(X_n=j)=\pi_j$, π_j stationary distribution

Considered $Y_n = X_{N-n}$ $n=0,\dots,N$

Y_n is also a Markov chain and has transition probabilities $Q_{ij}=\frac{\pi_j}{\pi_i}\cdot P_{ji}$

Definition If $P_{ij}=\frac{\pi_j}{\pi_i}P_{ji}$ the Markov chain is time reversible.

alternatively the condition is $\pi_i P_{ij}=\pi_j P_{ji}$

Remark 4.8.1 $\pi_i P_{ij}$ is the rate where the backward chain moves from i to j

$\pi_j P_{ji}$ is the rate for which the forward chain moves from j to i.

That these two rates are equal is a strong assumption.

Lemma. If $\exists \{x_j\}$ $x_j \geq 0$ $\sum x_i = 1$

and $x_i P_{ij} = x_j P_{ji}$ all i,j

then $x_i = \sum_j x_j P_{ji}$ so

$x_i = \pi_i$ where π_i are the stationary or limiting probabilities.

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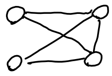
Proof. $\sum_j x_j P_{ji} = \sum_j x_i P_{ij} = x_i \sum_j P_{ij} = x_i$

So since π is unique for ergodic chains

$x_i = \pi_i$ all i ∎

Exmple Random walk on a graph.



Random walk on a graph: Pick a node, then move to the next by picking a neighbor at random

Let $d_i = \#$ neighbor at node i

$d=\sum d_i$, $P_{ij}=\frac{1}{d_i}$ $j=1,\dots,d_i$

Let $\pi = \left(\frac{d_1}{d},\dots,\frac{d_N}{d}\right)$ $N=\#$ nodes.

Is the chain reversible?

$$\pi_i \cdot P_{ij} = \begin{cases} \frac{d_i}{d}\cdot\frac{1}{d_i} = \frac{1}{d} & i,j \text{ neighbors} \\ 0 & \text{else}\end{cases}$$

$$\pi_j P_{ji} = \begin{cases} \frac{d_j}{d}\cdot\frac{1}{d_j} = \frac{1}{d} & i,j \text{ neighbors} \\ 0 & \text{else}\end{cases}$$

Hence random walk on a graph is time reversible.

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4.9 Markov Chain Monte Carlo (MCMC)

Consider X discrete and take values at $\{0,1,2,\dots$

Want $E\,h(X)$ some h.

One option. Simulate independent $X_1, X_2, \dots$

$$\lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} h(X_i) \to E\,h(X)$$ under

weak regularity by law large numbers.

Although in principle possible this can be difficult for complicated distribution of X.

Other option: Recall

Proposition 4.6 p 417 If X_n is irreducible Markov chain with stationary probabilities π_j, $j=0,1,\dots$. Then for r bounded $\lim \frac{1}{N}\sum_{n=1}^{N} r(X_n) \to \sum_{j=0}^{\infty} r(j)\cdot\pi_j$

Thus if we can find a Markov chain X_n with stationary probabilities $\lim_{n\to\infty} P(X_n=j)=\pi_j$

$$E\,h(X) = \sum h(j)P(X=j) = \sum_{j=0}^{\infty} h(j)\cdot\pi_j = \lim \frac{1}{N}\sum_{n=1}^{N} h(X_n)$$

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The aim is therefore to construct Markov chain having the specified probabilities as stationary distribution.

We will consider the case where $\pi_j = C\cdot b_j$ where b_j, $j=1,2,\dots$ are specified but C is unspecified.

Let $Q=\{q(i,j)\}_{j=1}^{\infty}$ be any specified Markov transition matrix on the integers

$q(x_j,\cdot)$ is called a proposal distribution, and should be easy to simulate.

Use the algoritm 1. For $X_n=i$ generate Y

$P(Y=j)=q(i,j)$

2. If $Y=j$

$$X_{n+1} = \begin{cases} j & \text{with probability } \alpha(i,j) \\ i & \text{---"---}\ 1-\alpha(i,j)\end{cases}$$

where $\alpha(i,j)$ is the acceptance probability (to be specified)

Remark 4.9.1 Possible for the chain X_n to remain in state i, i.e. $X_n=i$

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Now X_n has transition probability

$$P_{ij}=P(X_{n+1}=j\,|\,X_n=i) = \begin{cases} q(i,j)\cdot\alpha(i,j) & i\neq j \\ q(i,i)+\sum_{k\neq i} q(i,k)(1-\alpha(i,k)) \end{cases}$$

Since

$$\sum_{j\neq i} P_{ij} + P_{ii} = \sum_{j\neq i} \cancel{q(i,j)\alpha(i,j)} + \underbrace{q(i,i) + \sum_{k\neq i} q(i,k)}_{=1} - \sum_{k\neq i} \cancel{q(i,k)}\alpha(i,k)$$

Is this chain, X_n, time revercible?

i.e. $\pi(i)P_{ij} = \pi(j)P_{ji}$ $j\neq i$ or

(*) $\pi(i)\,q(i,j)\,\alpha(i,j) = \pi_j\,q(j,i)\,\alpha(j,i)$ $j\neq i$

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Lemma: Let $\alpha(i,j) = \min\left\{\frac{\pi(j)\,q(j,i)}{\pi(i)\,q(i,j)}, 1\right\}$

then (*) is satisfied.

Proof. $\alpha(i,j) = \min\left\{\frac{\pi(j)\,q(j,i)}{\pi(i)\,q(i,j)}; 1\right\}$

$\alpha(j,i) = \min\left\{\frac{\pi(i)\,q(i,j)}{\pi(j)\,q(j,i)}, 1\right\}$

(1) $\alpha(i,j) = \frac{\pi(j)\cdot q(j,i)}{\pi(i)\ q(i,j)} < 1$

$\Rightarrow \frac{\pi(i)\,q(i,j)}{\pi(j)\,q(j,i)} > 1$ and $\alpha(j,i)=1$

So

$$\pi(i)q(i,j)\,\alpha(i,j) = \pi(i)q(i,j)\left[\frac{\pi(j)\,q(j,i)}{\pi(i)\,q(i,j)}\right] = \pi(j)q(j,i)\cdot 1 = \pi(j)q(j,i)\cdot\alpha(j,i)$$

i.e (*)

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(*) Now consider $\alpha(i,j) < 1$

$$\Rightarrow \frac{\pi(j)\,q(j,i)}{\pi(i)\,q(i,j)} > 1$$

$$\Rightarrow \frac{\pi(i)\,q(i,j)}{\pi(j)\,q(j,i)} < 1$$

$$\Rightarrow \alpha(j,i) = \frac{\pi(i)\,q(i,j)}{\pi(j)\,q(j,i)}$$

$$\Rightarrow \pi(i)\,q(i,j)\cdot \underbrace{\alpha(i,j)}_{=1} = \pi(i)\cdot q(i,j) = \pi(j)\cdot q(j,i)\cdot \alpha(j,i) \quad \text{i.e. } (*)$$

Consider now $\pi(j) = \frac{b(j)}{B}$ $b(j)$ specified, B unspecified.

then $\alpha(i,j) = \min\left\{ \frac{b(j)\,q(j,i)}{b(i)\,q(i,j)}, 1 \right\}$ since B cancels in.

Remark 4.9.2 Usually $\pi(j)$ are not only stationary probabilities but will also be limiting probabilities. The condition $P_{ii} > 0$ will suffice. The the chain cannot be aperiodic.

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Example Permutations of $\{1, \dots, n\}$ $(x_1, \dots, x_n)$

$$\mathcal{S} = \left\{ (x_1, \dots, x_n) : \sum_{j=1}^{n} j\,x_j > a \right\} \quad a > \text{given}.$$

How big is $\mathcal{S}$? Want to construct a Markov chain with $\pi_j = \frac{1}{\#\mathcal{S}}$ $\#\mathcal{S}$ = number of elements in $\mathcal{S}$.

Each permutation in $\mathcal{S}$ is a node in a graph. Two ~~graphs~~ nodes are connected if only two elements are changed ex. $(1,2,3,4)$ and $(1,2,4,3)$ are connected but not $(1,2,3,4)$ $(1,3,4,2)$.

Proposal distribution: Let $N(\underline{s})$ be the neighbors of $\underline{s}$ and $\#N(s)$ the number of neighbors.

$$q(\underline{s},\underline{t}) = \frac{1}{\#N(\underline{s})} \quad t \in N(\underline{s})$$

Since $\pi_j = \frac{1}{\#\mathcal{S}}$ $\pi(\underline{s}) = \pi(\underline{t})$. Then $\alpha(\underline{s},\underline{t}) =$

$$\min\left\{ \frac{q(\underline{t},\underline{s})}{q(\underline{s},\underline{t})}, 1 \right\} = \min\left\{ \frac{\#N(\underline{s})}{\#N(\underline{t})}, 1 \right\}$$

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