

Markov Chains and Applications

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Abstract

In this paper I provide a quick overview of Stochastic processes and then quickly delve into a discussion of Markov Chains. There is some assumed knowledge of basic calculus, probability, and matrix theory. I build up Markov Chain theory towards a limit theorem. I prove the Fundamental Theorem of Markov Chains relating the stationary distribution to the limiting distribution. I then employ this limiting theorem in a MCMC example.

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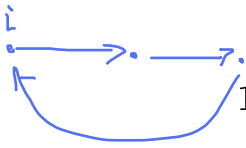
$N_i := \sum I\{X_n = i\}$ the
number of state i in the chain

Lemma. $P(N_i \geq k | X_0 = i) = P(T_i < \infty | X_0 = i) \wedge k$
 $P(N_i = k | X_0 = i) = P(T_i < \infty | X_0 = i) \wedge \{k\} P(T_i = \infty | X_0 = i)$

Fact.

$N_i \geq k = T_i(k) < \infty$ k -th hitting time

$N_i = k = T_i(k) < \infty$ and $T_i(k+1) = \infty$



1 Introduction

$E(N_i) = \sum p_{ii}(n) = P(T_i < \infty | X_0 = i) / P(T_i = \infty | X_0 = i)$

$P_i(T_i(2) = T_i(1) + n | T_i(1) < \infty)$
 $= P_i(T_i(1) = n)$

In a deterministic world, it is good to know that sometimes randomness can still occur. A stochastic process is the exact opposite of a deterministic one, and is a random process that can have multiple outcomes as time progresses. This means that if we know an initial condition for the process and the function by which it is defined, we can speak of likely outcomes of the process. One of the most commonly discussed stochastic processes is the Markov chain. Section 2 defines Markov chains and goes through their main properties as well as some interesting examples of the actions that can be performed with Markov chains. The conclusion of this section is the proof of a fundamental central limit theorem for Markov chains. We conclude the discussion in this paper by drawing on an important aspect of Markov chains: the Markov chain Monte Carlo (MCMC) methods of integration. While we provide an overview of several commonly used algorithms that fall under the title of MCMC, Section 3 employs importance sampling in order to demonstrate the power of MCMC.

2 Markov Chains

Markov chains are stochastic processes that have the Markov Property.

Definition of Markov Property Informally it is the condition that given a state, the past and future states are independent of it. Formally

$$\mathbb{P}(X_n = x | X_0, \dots, X_{n-1}) = \mathbb{P}(X_n = x | X_{n-1}) \quad \forall n \forall x.$$

2.1 Theorems and lemmas

notation: P always represents a transition matrix, p_{ij} represents an element of it.

Definition State i is **recurrent** if

$$\mathbb{P}(X_n = i \text{ for some } n \geq 1 | X_0 = i) = 1.$$

Otherwise it is **transient**.

Definition A chain is **irreducible** if every state can be reached from any other one. That is $p_{ij}(1) > 0 \forall i, j$ **$p_{ii} > 0$, i : aperiodic**

Fact.

A state is recurrent if and only if $\sum_n p_{ii}(n) = \infty$ and it is transient if and only if $\sum_n p_{ii}(n) < \infty$.²

$$\sum p_{ji}(n) = \infty, \text{ for all } j \rightarrow i$$

$$p_{ij}(n) := P(X_n = j | X_0 = i)$$

$$P(n) = P^n, \text{ homogeneous}$$

Fact. i : recurrent iff

$X_n = i$, for some n ; $\cup_n \{X_n = i\}$;

$T_i < \infty$, i-a.s. (T_i : hitting time from i to i)

$N_i = \infty$, i-a.s.

$j \rightarrow i$ iff $p_{ji}(n) > 0$ for some n

Lemma 2.1 *In an irreducible chain, all the states are either transient or recurrent.*

Proof We take the shortest path from state i to state j (let it have n steps), and the shortest path from j to i (let it have m steps). Thus we have $p_{ij}(n) = a > 0$ and $p_{ji}(m) = b > 0$ and so we have

$$\begin{aligned} p_{ii}(l+n+m) &\geq p_{ij}(n) p_{jj}(l) p_{ji}(m) \\ &= ab p_{jj}(l) \\ p_{jj}(l+n+m) &\geq p_{ji}(m) p_{ii}(l) p_{ij}(n) \\ &= ab p_{ii}(l). \end{aligned}$$

Fact. $i \leftrightarrow j$
1. $p_{ii}(l+k) \geq p_{jj}(l); p_{jj}(l+k) \geq p_{ii}(l)$
2. $p_{ii}(l) \sim p_{jj}(l)$

So it is obvious that either $\sum_n p_{ii}(n)$ and $\sum_n p_{jj}(n)$ are both finite or are both infinite. Thus from the above results we note that all the states of an irreducible chain are either transient or recurrent, as desired.

Lemma 2.2 *Facts about recurrence.*

1. If $i \leftrightarrow j$, then ij recurrent. or i, j transient.
2. The states of a finite, irreducible Markov chain are all recurrent.

$$= E T_i$$

Definition Mean recurrence time for a recurrent state i is $m_i = \sum_n n f_{ii}(n)$ where $f_{ii}(n)$ is the probability of getting from i to i in exactly n steps. A state is null recurrent if $m_i = \infty$ and non-null positive otherwise. the distr. of hitting time T_i

fact a finite state Markov chain has all its recurrent states be non-null.

Definition The period of state i , $d(i) = d$ if $p_{ii}(n) = 0$ for $d \nmid n$ and $d = \gcd\{n | p_{ii}(n) > 0\}$. Thus a state is periodic if $d(i) > 1$ and aperiodic otherwise.

Definition For $\pi_i = \lim_{n \rightarrow \infty} p_{ii}(n \times d(i))$, if greater than zero then non-null recurrent otherwise, null recurrent. $\pi_i = \lim_{n \rightarrow \infty} p_{ii}(n)$ for large n , $p_{ii}(n) > 0$

Lemma 2.3 If $i \leftrightarrow j$ then $d(i) = d(j)$

Proof We consider m, n st $p_{ij}(n) > 0$ and $p_{ji}(m) > 0$ thus we can note that from the Kolmogorov Chapman equations we have

$$p_{ii}(m+n) \geq p_{ij}(n) p_{ji}(m).$$

Now by definition $p_{ii}(n+m) > 0$ and $d(i) | (n+m)$.

$$p_{ii}(m+l+n) \geq p_{ij}(n) p_{jj}(l) p_{ji}(m)$$

So if we have that $p_{jj}(l) > 0$ then $d(j) | l$ implying as desired that $p_{ii}(m+l+n) > 0$ and so $d(i) | (n+m+l)$ but combining this with $d(i) | (m+n)$ we get that $d(i) | l$ and so since $d(j) = \gcd\{l | p_{jj}(l) > 0\}$ we get that $d(j) \geq d(i)$.

$$\implies d(i) = d(j)$$

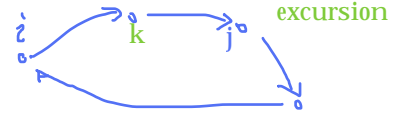
Definition A chain is ergodic if all of its states are non-null recurrent and aperiodic.

Definition Let π be a pmf, then we say that π is a stationary probability distribution if $\pi = \pi P$ (π is an eigenvector of the P)

Definition A limiting distribution exists if $P^n \rightarrow \begin{bmatrix} \pi \\ \vdots \\ \pi \end{bmatrix}$ for some π

Theorem. Recurrent & Irreducible \implies E! unique stationary distr.

$$\begin{aligned}\pi_j &\sim \mathbb{E} \#\{X_t = j, 0 \leq t < T_i\}, j = 0, 1, \dots \\ &= \sum_{0 \leq t < T_i} \mathbb{P}(X_t = j) \\ &= \sum_{0 \leq t < T_i-1, k} \mathbb{P}(X_t = k) \mathbb{P}(j | k) \\ &= \sum_k \left(\sum_{0 \leq t < T_i} \mathbb{P}(X_t = k) \right) \mathbb{P}(j | k) \quad (\text{recurrent})\end{aligned}$$



Theorem 2.4 (Fundamental theorem for Markov Chains) *An irreducible, ergodic Markov chain has a unique stationary distribution π = The limiting distribution.*

Proof Since the chain is ergodic, it is non-null recurrent which implies from above that $\pi_j = \lim_{n \rightarrow \infty} p_{ij}(n) > 0 \forall i$ and $\sum \pi_j = 1$. /

by Fatou lemma

$$\implies \pi_i \geq \sum_k \pi_k p_{ki}.$$

Now we assume the inequality is strict for some i which leads to the following contradiction:

$$\sum_{i=0}^{\infty} \pi_i \geq \sum_{i=0}^{\infty} \sum_{k=0}^{\infty} \pi_k p_{ki} = \sum_{k=0}^{\infty} \pi_k.$$

Thus we come to the conclusion that $\pi_i = \sum_{k=0}^{\infty} \pi_k p_{ki} \forall i$. Now we can consider $\tilde{\pi}_i = \pi_i / \sum_{k=0}^{\infty} \pi_k$ to be a stationary distribution. So we have shown existence.

Now to show uniqueness :
by Fatou lemma

$$\tilde{\pi}_i = \mathbb{P}(X_n = i) = \sum_{j=0}^{\infty} \mathbb{P}(X_n = i | X_0 = j) \mathbb{P}(X_0 = j) = \sum_{j=0}^{\infty} p_{ji}(n) \tilde{\pi}_j.$$

Now we know that $\tilde{\pi}$ is a stationary distribution so it sums up to 1, we get $\tilde{\pi}_i \leq \sum_j \pi_j \tilde{\pi}_j = \pi_i$

\implies that the stationary distribution is unique.

the existence of a limiting distribution and so we now know that an ergodic chain converges to its stationary distribution.

take any bounded function g and say with probability 1 that

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N g(X_n) \rightarrow E_{\pi}(g) \equiv \sum_j g(j) \pi_j$$

Definition π satisfies detailed balance if $\pi_i p_{ij} = p_{ji} \pi_j$ DBC

Lemma 2.5 *If π satisfies detailed balance then it is a stationary distribution.*

P

3 Markov Chain Monte Carlo

Markov chain Monte Carlo integration is a method for integrating function that might not have a closed form using estimation.

We demonstrate a very basic example of MCMC processes through Importance Sampling. Importance sampling is used in statistics as a variance reduction method. While the standard method that we describe below does not necessarily optimize the variance, we will state the condition for minimal variance. Importance sampling allows us to estimate the distribution of a rv using a different rv. The idea behind the process is that during the simulation, due to weighing of the rv from which we have the observations, we get a better, less biased idea of the parameter we are estimating. Thus the choice of the weight is very important. We will not go through the derivation of the “best” (in terms of minimizing the variance) weight, but just state the result here.

In an importance sampling problem we are trying to estimate the distribution of I using $\hat{I} = \frac{1}{N} \sum \frac{h(X_i)f(X_i)}{g(X_i)}$. The optimal choice of g in this case is $g(x) = \frac{|h(x)|f(x)}{\int |h(s)|f(s)ds}$.

3.1 Statement

(From Larry Wasserman's All of Statistics, 24.7.2)

Let $f_{X,Y}(x,y)$ be a bivariate density and let $(X_1, Y_1), \dots, (X_N, Y_N) \sim f_{X,Y}$.

1. Let $w(x)$ be an arbitrary pdf. Let

$$\hat{f}_X(x) = \frac{1}{N} \sum_{i=1}^N \frac{f_{X,Y}(x, Y_i) w(x)}{f_{X,Y}(X_i, Y_i)}.$$

Show that, for each x , $\hat{f}_X(x) \xrightarrow{P} f_X(x)$. Find an expression for the variance.

2. Let $Y \sim N(0, 1)$ and $X|Y = y \sim N(y, 1 + y^2)$. Use the method in (1) to estimate $f_X(x)$.

3.2 Solution

1. We consider each part of the sum to be its own rv, and we note that they are all iid. Due to this we can consider just one of them for the following:

$$\begin{aligned} E \left[\frac{f_{X,Y}(x, Y_i) w(x)}{f_{X,Y}(X_i, Y_i)} \right] &= \int \frac{f_{X,Y}(x, y) w(x)}{f_{X,Y}(z, y)} f_{X,Y}(z, y) dz dy \\ &= f_X(x) \end{aligned}$$

and so we can apply the law of large numbers

$$\frac{1}{N} \sum_{i=1}^N \frac{f_{X,Y}(x, Y_i) w(x)}{f_{X,Y}(X_i, Y_i)} \xrightarrow{P} E \left[\frac{f_{X,Y}(x, Y_i) w(x)}{f_{X,Y}(X_i, Y_i)} \right]$$

which is the same as $\hat{f}_X(x) \xrightarrow{P} f_X(x)$, as desired.

The variance calculation is fairly simple and we do not dwell on it, providing simply the easily verifiable answer:

$$\text{var} \hat{f}_X(x) = \frac{1}{N} \left[\int \frac{f_{X,Y}^2(x, y) w^2(y)}{f_{X,Y}(x, y)} dy - f_X^2(x) \right].$$

2. We note that the marginal density of X is hard to evaluate:

$$\begin{aligned} f_X(x) &= \int f_{X|Y}(x|y) f_Y(y) dy \\ &= \int \frac{1}{\sqrt{2\pi(1+y^2)}} e^{-\frac{(x-y)^2}{2(1+y^2)}} \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}} dy. \end{aligned}$$

Thus it makes sense to employ importance sampling as in (1) in order to estimate $f_X(x)$. So we take the distribution of $w(x)$ to be the Standard Normal as it seems like a reasonable one in this case. So we have:

$$\begin{aligned} \hat{f}_X(x) &= \frac{1}{N} \sum_{i=1}^N \frac{f_{X,Y}(x, Y_i) w(x)}{f_{X,Y}(X_i, Y_i)} \\ &= \frac{1}{N} \sum_{i=1}^N \frac{f_{X|Y}(x|Y_i) w(X_i)}{f_{X|Y}(X_i|Y_i)} \\ &= \frac{1}{N} \sum_{i=1}^N \frac{1}{\sqrt{2\pi}} \exp \left\{ -\frac{1}{2(1+Y_i^2)} \left[(x - Y_i)^2 - (X_i - Y_i)^2 + (X_i(1+Y_i^2))^2 \right] \right\} \end{aligned}$$

3.3 Further Discussion

We see above a very basic application of MCMC methods which allows us to use a biased sampling distribution in order to estimate a r.v. of interest. The above discussed method is a very basic and introductory one. We actually have multiple possible algorithms that we can apply in order to arrive at the best possible estimate, however they are a topic for another paper and will only be briefly mentioned here.

The most commonly used algorithms for MCMC are the Metropolis Hastings algorithms which use a conditional proposal distribution in order to construct a Markov chain with a stationary distribution f . It supposes that X_0 was chosen arbitrarily and then proceeds to use the proposal distribution in order to

generate candidates that are either added to the chain or are overlooked based on a specified probability distribution.⁴ There are several different incarnations of this algorithm, with different suggested proposal distributions: the random-walk M-H algorithm is the one that was described above (as if we do not accept or reject the generated value, all we are doing is simulating a random walk on the real line). In independence M-H we change the proposal distribution to a fixed distribution which we believe to be an approximation of f .

Another method that gets a lot of use is the Gibbs sampling algorithm which is simply an embellishment of the M-H algorithm. What this method does is take a multi-dimensional problem and turns it into several one-dimensional problems that can be easily estimated using the above method. So instead of simply getting X_{i+1} , Gibbs sampling allows for the estimation of $(X_{i+1}^{(1)}, \dots, X_{i+1}^{(n)})$ for an n -dimensional model.

This process works due to detailed balance of Markov Chains, which was briefly mentioned in the previous section. For further information consult Wasserman's book.

⁴For basic Metropolis-Hastings, we have the probability be $r(x, y) = \min \left\{ \frac{f(y) q(x|y)}{f(x) q(y|x)}, 1 \right\}$ where q is the proposal distribution. In the case that we have, we can easily choose a q such that $q(x|y) = q(y|x)$ so obviously one part of the multiplication cancels out.