## Chapters 2 and 3: Discrete-Time Markov Chains (DTMCs)

Transition probabilities:

$$
p_{j i}(n)=\operatorname{Prob}\left\{X_{n+1}=j \mid X_{n}=i\right\}
$$

If $p_{j i}(n)$ does not depend on $n$, then the process is said to be time homogeneous. The transition matrix of a DTMC $\left\{X_{n}\right\}_{n=0}^{\infty}$ with state space $\{1,2, \ldots\}$ and one-step transition probabilities, $\left\{p_{i j}\right\}_{i, j=1}^{\infty}$, is denoted as $P=\left(p_{i j}\right)$, where

$$
P=\left(\begin{array}{cccc}
p_{11} & p_{12} & p_{13} & \cdots \\
p_{21} & p_{22} & p_{23} & \cdots \\
p_{31} & p_{32} & p_{33} & \cdots \\
\vdots & \vdots & \vdots &
\end{array}\right) .
$$

The column sums equal one, a stochastic matrix, $\sum_{j=1}^{\infty} p_{j i}=1$. The $n$-step transition matrix $P^{n}=\left(p_{i j}^{(n)}\right)$. The probabilities $p_{i}(n)=\operatorname{Prob}\left\{X_{n}=i\right\}, p_{i}(n+1)=\sum_{j=1}^{\infty} p_{i j} p_{j}(n), i=1,2 \ldots$

$$
p(n+1)=P p(n)
$$

Random walk model with absorbing barriers. See the directed graph in Figure 1 and the corresponding $(N+1) \times(N+1)$ transition matrix:

$$
P=\left(\begin{array}{ccccccc}
1 & q & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & q & \cdots & 0 & 0 & 0 \\
0 & p & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & p & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & q & 0 \\
0 & 0 & 0 & \cdots & p & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & p & 1
\end{array}\right) .
$$

The Markov chain, graphed in Figure 1, has three communication classes: $\{0\},\{1,2, \ldots, N-1\}$, and $\{N\}$. The Markov chain is reducible. States 0 and $N$ are absorbing; the remaining states are transient.


Figure 1: Probability of moving to right is $p$ and to the left is $q, p+q=1$. Boundaries 0 and $N$ are absorbing, $p_{00}=1=p_{N N}$ (random walk with absorbing barriers or gambler's ruin problem).

A DTMC is irreducible if its digraph is strongly connected. Otherwise it is called reducible. An irreducible DTMC can be positive recurrent or null recurrent or transient. It may also be classified as periodic or aperiodic. Recurrence is defined for each state $i$ in the chain. Recurrence means for each state $i$ if the process leaves state $i$ it will return to state $i$ at some future time. If not, the state is transient. A state $i$ is positive recurrent if the mean recurrence time ( $\mu_{i i}$ mean return time) is finite. A state $i$ with an infinite mean recurrence time is called null recurrent. Periodicity and recurrence are class properties. That means, the entire communicating class will have the same period (or be aperiodic) and same recurrence (either positive recurrent or null recurrent). An example of a null recurrent process is the symmetric random walk on the set of integers.

An ergodic Markov chain is a Markov chain that is irreducible, aperiodic and positive recurrent. An irreducible finite Markov chain is always positive recurrent. Thus, an irreducible, aperiodic finite Markov chain is ergodic. The following theorem shows the importance of ergodic chains. The following theorems apply to null recurrent and positive recurrent chains.

Theorem 1 (Basic Limit Theorem for aperiodic Markov chains) Let $\left\{X_{n}\right\}_{n=0}^{\infty}$ be a recurrent, irreducible, and aperiodic DTMC with transition matrix $P=\left(p_{i j}\right)$. Then

$$
\lim _{n \rightarrow \infty} p_{i j}^{(n)}=\frac{1}{\mu_{i i}},
$$

where $\mu_{i i}$ is the mean recurrence time for state $i$ and $i$ and $j$ are any states of the chain. [If $\mu_{i i}=\infty$, then $\lim _{n \rightarrow \infty} p_{i j}^{(n)}=0$.]

The first theorem states that there exists a limit of $P^{n}$ and, in particular, the columns of the limiting matrix $P^{n}$ are all the same. In fact, the limiting column is the limiting stationary distribution $p(n) \rightarrow \pi$, provided the DTMC is ergodic. That is,

$$
\lim _{n \rightarrow \infty} p(n)=\lim _{n \rightarrow \infty} P^{n} p(0)=P_{\infty} p(0)=\pi
$$

where all of the columns of $P_{\infty}$ are $\pi=\left(\pi_{1}, \pi_{2}, \ldots\right)^{t r}$, where $\pi_{i}>0$ (hence the term positive recurrent). For an ergodic finite Markov chain, the limiting stationary distribution can be found by computing the eigenvector corresponding to the eigenvalue 1 of $P: P \pi=\pi$, where $\sum \pi_{i}=1$. Also, $\mu_{i i}=\frac{1}{\pi_{i}}$.

The preceding theorem is extended to periodic chains.
Theorem 2 (Basic Limit Theorem for periodic Markov chains) Let $\left\{X_{n}\right\}_{n=0}^{\infty}$ be a recurrent, irreducible, and d-periodic DTMC, $d>1$, with transition matrix $P=\left(p_{i j}\right)$. Then

$$
\lim _{n \rightarrow \infty} p_{i i}^{(n d)}=\frac{d}{\mu_{i i}}
$$

and $p_{i i}^{(m)}=0$ if $m$ is not a multiple of $d$, where $\mu_{i i}$ is the mean recurrence time for state $i$. [If $\mu_{i i}=\infty$, then $\lim _{n \rightarrow \infty} p_{i i}^{(n d)}=0$.]

The random walk on $\{0, \pm 1, \pm 2, \ldots\}$ with probability moving to right equal to $p$ and to the left equal to $q$, with $p+q=1, p>0, q>0$, is an irreducible, 2-periodic DTMC. If $p=q=1 / 2$, then the DTMC is null recurrent and if $p \neq q$, then the DTMC is transient.

Random Walk with Absorbing Boundaries or Gambler's Ruin Let's return to the random walk model with absorbing boundaries. This DTMC does not satisfy either of the Basic Limit Theorems because it is a reducible Markov chain with three communicating classes, two absorbing states $\{0\}$ and $\{N\}$ and the transient class $\{1,2, \ldots, N-1\}$. Interesting questions about problems with absorbing states such as an extinction state in population dynamics are: (1) What is the probability of absorption? and (2): What is the expected time until absorption? We investigate this question with the random walk model and with the genetics of inbreeding for a finite DTMC. Later, we investigate the probability of extinction in a population model via a branching process.

Consider the random walk model with absorbing boundaries at 0 and $N$. In the gambler's ruin problem, state 0 is ruin and state N is winning the maximum amount of money. In either case, after hitting 0 or N , you stop playing the game. Let $a_{k}$ be the probability of ruin (absorption at $k=0$ ) beginning with a capital of $k$ :

$$
\begin{equation*}
a_{k}=p a_{k+1}+q a_{k-1} \tag{1}
\end{equation*}
$$

for $1 \leq k \leq N-1$. Equation (1) is a second-order difference equation in $a_{k}$. The difference equation can be written as

$$
\begin{equation*}
p a_{k+1}-a_{k}+q a_{k-1}=0, \quad k=1, \ldots, N-1 . \tag{2}
\end{equation*}
$$

This method of deriving equation (1) is referred to as a first-step analysis (Taylor and Karlin, 1998). This difference equation (2) can be solved with the following boundary conditions

$$
a_{0}=1 \text { and } a_{N}=0
$$

by assuming $a_{k}=\lambda^{k}$ with characteristic equation: $p \lambda^{2}-\lambda+q=0$. Alternately, it can be shown that there exists a submatrix $T$ of $P$ for the set of transient states, where matrix $T$ is not a stochastic matrix. In fact, matrix $T$ has the property that the spectral radius is $\rho(T)<1$ and therefore $(I-T)$ is invertible. The probability of absorption $a_{k}$ starting from state $k$ can be obtained as follows:

$$
\left(a_{1}, \ldots, a_{N-1}\right)=\left(p_{01}, p_{02}, \ldots, p_{0, N-1}\right)(I-T)^{-1}
$$

For a more general Markov chain with two absorbing states at 0 and $N$ for which there may be a probability of a transition from state $k$ to state $i, p_{i k}$ (jump from state $k$ to $i$ with probability $p_{i k}$ ), the difference equation from the first-step analysis for probability of absorption has the form:

$$
a_{k}=\sum_{k=0}^{N} p_{i k} a_{i} .
$$

To find the probability of absorption into state $N$, the boundary conditions are $a_{0}=0$ and $a_{N}=1$.
Expected Time until Absorption: Let $\tau_{k}$ be the mean time until absorption into either states 0 or N in the gambler's ruin problem. The difference equation for $\tau_{k}$ has the following form:

$$
\tau_{k}=p\left(1+\tau_{k+1}\right)+q\left(1+\tau_{k-1}\right),
$$

for $k=1,2, \ldots, N-1$ or

$$
\begin{equation*}
p \tau_{k+1}-\tau_{k}+q \tau_{k-1}=-1, \tag{3}
\end{equation*}
$$

The boundary conditions are $\tau_{0}=0=\tau_{N}$. An explicit solution to this difference equation with the boundary conditions can be solved by finding the general solution of the homogeneous difference equation and adding the particular solution of the nonhomogeneous equation, $\tau_{k}=$ homogeneous solution + particular solution. Alternately, it can be shown that the matrix $T$ can be used to compute the mean time until absorption from state $k, \tau_{k}$. In particular, It can be shown that

$$
\left(\tau_{1}, \tau_{2}, \ldots, \tau_{N-1}\right)=\mathbf{1}(I-T)^{-1}, \quad \mathbf{1}=(1,1, \ldots, 1)
$$

In a more general Markov chain with two absorbing states, the difference equation for the absorprion ttakes the form:

$$
\tau_{k}=\sum_{i=0}^{N} p_{i k}\left(1+\tau_{i}\right) \quad \text { or } \quad \tau_{k}-\sum_{i=0}^{N} p_{i k} \tau_{i}=1
$$

Table 1: Gambler's ruin problem with a beginning capital of $k=50$ and a total capital of $N=100$

| Prob. | $a_{50}$ | $b_{50}$ | $\tau_{50}$ | $A_{50}^{\prime}(1)$ | $B_{50}^{\prime}(1)$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $q=0.50$ | 0.5 | 0.5 | 2500 | 1250 | 1250 |
| $q=0.51$ | 0.880825 | 0.119175 | 1904 | 1677 | 227 |
| $q=0.55$ | 0.999956 | 0.000044 | 500 | 499.93 | 0.07 |
| $q=0.60$ | 1.00000 | 0.00000 | 250 | 250 | 0 |



Figure 2: Three sample paths for the gambler's ruin problem when $N=100, k=50$, and $q=0.55$

Example of Genetics of Inbreeding: Two alleles $A$ and $a$. There are six possible breeding pairs which denote the six states of the DTMC, 1: $A A \times A A, 2$. $a a \times a a, 3 . A a \times A a, 4 . A a \times a a, 5 . A A \times a a, 6$. $A A \times A a$. Inbreeding of the first two types results in offspring of the same genotypes and inbreeding in the next generation will be of the same type; they are absorbing states. The remaining states, $3,4,5,6$ are transient. The transition matrix has the following form:

$$
P=\left(\begin{array}{cccccc}
1 & 0 & 1 / 16 & 0 & 0 & 1 / 4 \\
0 & 1 & 1 / 16 & 1 / 4 & 0 & 0 \\
0 & 0 & 1 / 4 & 1 / 4 & 1 & 1 / 4 \\
0 & 0 & 1 / 4 & 1 / 2 & 0 & 0 \\
0 & 0 & 1 / 8 & 0 & 0 & 0 \\
0 & 0 & 1 / 4 & 0 & 0 & 1 / 2
\end{array}\right)=\left(\begin{array}{cc}
I & A \\
O & T
\end{array}\right)
$$

Probability of absorption into states 1 or 2 from states $3,4,5,6$ is computed from the fundamental matrix, $(I-T)^{-1}$,

$$
\lim _{n \rightarrow \infty} P^{n}=\left(\begin{array}{cc}
I & \left(A+A T+A T^{2}+\cdots\right) \\
O & O
\end{array}\right)=\left(\begin{array}{cc}
I & A(I-T)^{-1} \\
O & O
\end{array}\right)
$$

Thus, $A(I-T)^{-1}$ is the probability of absorption into states 1 or 2 (fixation) from states $3,4,5$ or 6 . Let $\mathbf{1}=(1,1,1,1)$, then $\mathbf{1}(I-T)^{-1}$ is the mean time until absorption from states $3,4,5$, or 6 .

