MTH 7241 Fall 2022: Prof. C. King

Notes 4: Finite Markov chains

A. A. Markov

Andrei Andreyevich Markov (1856 - 1922) founded the modern theory of stochastic processes, and gave his name to the special class we will consider here. He was an early activist for human rights in Imperial Russia, and in 1912 he protested Leo Tolstoy's excommunication from the Russian Orthodox Church. Markov was undaunted by extensive calculations and was very good at them. In what has now become the famous first application of Markov chains, A. A. Markov studied the sequence of 20,000 letters in A. S. Pushkins poem "Eugeny Onegin", discovering that the stationary vowel probability is $p = 0.432$, that the probability of a vowel following a vowel is $p_1 = 0.128$, and that the probability of a vowel following a consonant is $p_2 = 0.663$.

Markov chains

Markov's great contribution was the systematic analysis of a class of sequences of random variables $X_1, X_2, \dots$ which are dependent, but only in the simplest possible way. In a sense they are the nearest to independent chains. Thus for example the sequence of random steps $S_1, S_2, \dots$ is independent, while the random walk $\{X_k = S_1 + \cdots + S_k\}$ is not independent. However they are both Markov chains.

The theory has an enormous range of applications, including:

- statistical physics
- queueing theory
- communication networks
- voice recognition
- bioinformatics
- Google's pagerank algorithm
- computer learning and inference
- economics
- gambling
- data compression

$\boxed{\textbf{Definition of the chain}}$

Let Ω be a finite or countably infinite sample space. A collection of Ω-valued random variables $\{X_0, X_1, X_2, \ldots\}$ is called a discrete-time Markov chain on Ω if it satisfies the *Markov condition*:

$$P(X_{n+1} = j \mid X_0 = i_0, \ldots, X_n = i_n) = P(X_{n+1} = j \mid X_n = i_n) \tag{1}$$

for all $n \geq 0$ and all states $j, i_0, \ldots, i_n \in \Omega$.

Regarding the index of X_n as a discrete time the Markov condition can be summarized by saying that the conditional distribution of the future state X_{n+1} conditioned on the present and past states $X_0, \ldots, X_n$ is equal to the conditional distribution of X_{n+1} conditioned on the present state X_n. In other words, the future (random) behavior of the chain only depends on where the chain sits right now, and not on how it got to its present position.

We say that

$$P(X_{n+1} = j \mid X_n = i)$$

is the *transition probability* from state i to state j after n steps. We will mostly consider homogeneous chains, meaning that the transition probabilities do not depend on n. In this case for all n and $i, j \in \Omega$

$$P(X_{n+1} = j \mid X_n = i) = P(X_1 = j \mid X_0 = i) = p_{ij} \tag{2}$$

This defines the transition matrix P with entries p_{ij}. Any transition matrix P must satisfy these properties:

(P1) $p_{ij} \geq 0$ for all $i, j \in \Omega$

(P2) $\sum_{j \in \Omega} p_{ij} = 1$ for all $i \in \Omega$

Such a matrix is also called row-stochastic. So a square matrix is a transition matrix if and only if it is non-negative and row-stochastic.

An equivalent way to state the Markov condition is for any sequence of states $i, j, k, l, \ldots,$

$$P(X_0 = i, \ldots, X_1 = j, X_2 = k, X_3 = l, \ldots) = P(X_0 = i)\, p_{ij}\, p_{jk}\, p_{kl}, \ldots$$

Example 1 *Consider the following model. There are four balls, two White and two Black, and two boxes. Two balls are placed in each box. The transition mechanism is that at each time unit one ball is randomly selected from each box, these balls are exchanged, and then placed back into the boxes. Let X_n be the number of White balls in the first box after n steps. The state space is $S = \{0, 1, 2\}$. The transition matrix is*

$$P = \begin{pmatrix} 0 & 1 & 0 \\ 1/4 & 1/2 & 1/4 \\ 0 & 1 & 0 \end{pmatrix} \tag{3}$$

Why is it a Markov chain? The transition mechanism only depends on the current state of the system. Once you know the current state (= number of balls in first box) you can calculate the probabilities of the next state.

Once the initial probability distribution of X_0 is specified, the joint distribution of the future X_i is determined by the transition matrix. So let $\alpha_i = P(X_0 = i)$ for all $i \in \Omega$, then for any sequence of states $i_0, i_1, \ldots, i_m$ we have

$$P(X_0 = i_0, X_1 = i_1, \ldots, X_m = i_m) = \alpha_{i_0} p_{i_0,i_1} p_{i_1,i_2} \ldots p_{i_{m-1},i_m} \tag{4}$$

The transition matrix contains the information about how the chain evolves over successive transitions. For example,

$$\begin{aligned}
P(X_2 = j | X_0 = i) &= \sum_k P(X_2 = j, X_1 = k | X_0 = i) \\
&= \sum_k P(X_2 = j | X_1 = k, X_0 = i)\, P(X_1 = k | X_0 = i) \\
&= \sum_k P(X_2 = j | X_1 = k)\, P(X_1 = k | X_0 = i) \\
&= \sum_k p_{kj}\, p_{ik} \\
&= \sum_k (P)_{ik}\, (P)_{kj} \\
&= (P^2)_{ij} \qquad (5)
\end{aligned}$$

So the matrix P^2 provides the transition rule for two consecutive steps of the chain. It is easy to check that P^2 is also row-stochastic, and hence is the transition matrix for a Markov chain, namely the two-step chain $X_0, X_2, X_4, \ldots$, or $X_1, X_3, \ldots$. A similar calculation shows that for any $n \geq 1$

$$P(X_n = j | X_0 = i) = (P^n)_{ij} \tag{6}$$

and hence P^n is the n-step transition matrix. We write

$$p_{ij}(n) = (P^n)_{ij} = P(X_n = j | X_0 = i) \tag{7}$$

Note that $p_{ij} = 0$ means that the chain cannot move from state i to state j in one step. However it is possible in this situation that there is an integer n such that $p_{ij}(n) > 0$, meaning that it is possible to move from i to j in n steps. In this case we say that state j is *accessible* from state i.

Example 2 *For the balls in boxes example, all states are accessible from all other states.*

Example 3 *The drunkard's walk. The state space is* $\Omega = \{0, 1, 2, 3, 4\}$*, and* X_n *is the drunkard's position after* n *steps. At each step he goes left or right with probability* $1/2$ *until he reaches an endpoint* 0 *or* 4*, where he stays forever. The transition matrix is*

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{8}$$

Again the transition mechanism depends only on the current state, which means that this is a Markov chain. Are all states accessible from all other states?

A finite state Markov chain can be usefully represented by a directed graph where the vertices are the states, and edges are the allowed one-step transitions.

Classification of states

Define

$$f_{ij}(n) = P(X_1 \neq j, X_2 \neq j, \ldots, X_{n-1} \neq j, X_n = j \,|\, X_0 = i) \tag{9}$$

to be the probability that starting in state i the chain first visits state j after n steps. Define

$$\begin{aligned} f_{ij} &= \sum_{n=1}^{\infty} f_{ij}(n) \\ &= P(X_n = j \text{ for some } n \geq 1 \,|\, X_0 = i) \end{aligned}$$

This is the probability that the chain eventually visits state j starting in state i.

Definition 1 *The state j is* persistent *if $f_{jj} = 1$. The state j is* transient *if $f_{jj} < 1$.*

So the state j is persistent if the chain must eventually return to state j, given that it started at state j. Since the clock starts over at each return to state j, we conclude that if the state j is persistent then the chain must return to j infinitely often.

Similarly if j is transient, then the chain will return to state j only finitely often. Eventually it will never return to the state.

One particular type of persistent state is the class of *absorbing states*: these are the states for which $p_{ii} = 1$. So once the chain enters an absorbing state it can never leave. The end states of the drunkard's walk are absorbing states.

Deciding about persistence

There is a useful way to decide if a state is persistent or transient.

With the conventions $p_{ij}(0) = \delta_{ij}$ and $f_{ij}(0) = 0$, we have for each n

$$p_{ij}(n) = \delta_{ij}\, \delta_{n,0} + \sum_{k=1}^{n} f_{ij}(k)\, p_{jj}(n-k)$$

where we sum over k, the time of first visit to state j. This is a convolution formula so we can solve it by a transform. Define the generating functions

$$P_{ij}(s) = \sum_{n=0}^{\infty} s^n p_{ij}(n), \quad F_{ij}(s) = \sum_{n=0}^{\infty} s^n f_{ij}(n)$$

Then the convolution formula implies

$$P_{ij}(s) = \delta_{ij} + F_{ij}(s)\, P_{jj}(s)$$

For the case $i = j$ this yields

$$P_{ii}(s) = \frac{1}{1 - F_{ii}(s)}$$

Now consider what happens in the limit $s \to 1$. Recall Abel's theorem: if $a_n \geq 0$ for all n and $\sum_n a_n s^n$ is finite for all $|s| < 1$, then

$$\lim_{s \uparrow 1} \sum_{n=0}^{\infty} a_n s^n = \sum_{n=0}^{\infty} a_n$$

We apply this with

$$\lim_{s \uparrow 1} F_{ii}(s) = f_{ii}$$

We conclude that the state i is persistent ($F_{ii}(1) = 1$) if and only if

$$P_{ii}(1) = \sum_n p_{ii}(n) = \infty$$

So this is our useful test: the state i is persistent if and only if

$$\sum_{n=1}^{\infty} P(X_n = i \,|\, X_0 = i) = \infty$$

Classification of Markov chains

We say that the states i and j *intercommunicate* if there are integers n, m such that $p_{ij}(n) > 0$ and $p_{ji}(m) > 0$. In other words it is possible to go from each state to the other after a finite number of steps.

Theorem 1 *Suppose i, j intercommunicate, then they are either both transient or both persistent.*

Proof: Since i, j intercommunicate there are integers n, m such that

$$h = p_{ij}(n) p_{ji}(m) > 0 \tag{10}$$

Hence for any r,

$$p_{ii}(n + m + r) \geq p_{ij}(n) p_{jj}(r) p_{ji}(m) = h \, p_{jj}(r) \tag{11}$$

Sum over r to deduce

$$\sum_k p_{ii}(k) \geq \sum_r p_{ii}(n + m + r) \geq h \sum_r p_{jj}(r) \tag{12}$$

Therefore either both sums are finite or both are infinite, hence either both states are transient or both are persistent.

If all states intercommunicate we say that the Markov chain is *irreducible*.

A class of states C in Ω is called *closed* if $p_{ij} = 0$ whenever $i \in C$ and $j \notin C$.

There is a fairly obvious decomposition of the state space.
The state space Ω can be partitioned uniquely as

$$\Omega = T \cup C_1 \cup C_2 \cup \cdots \tag{13}$$

where T is the set of all transient states, and each class C_i is closed and irreducible.

If the chain starts with $X_0 \in C_i$ then it stays in C_i forever. If it starts with $X_0 \in T$ then eventually it enters one of the classes C_i and stays there forever. So the irreducible classes determine the *long-time behavior*.

Stationary distribution

Let $\{\pi_i\}$ $(i \in \Omega)$ be a probability distribution on Ω. We say that π_i is *stationary* if

$$\sum_i \pi_i \, p_{ij} = \pi_j$$

for all states $j \in \Omega$.

Lemma 1 *Suppose that $P(X_0 = j) = \pi_j$ for all $j \in \Omega$, where π is the stationary distribution. Then $P(X_n = j) = \pi_j$ for all $j \in \Omega$, and all $n \geq 1$.*

The proof is easy: note that

$$\begin{aligned} P(X_1 = j) &= \sum_i P(X_1 = j \,|\, X_0 = i) \, P(X_0 = i) \\ &= \sum_i p_{ij} \, \pi_i \\ &= \pi_j \end{aligned}$$

where we used the stationarity property in the last line.

Now repeat the argument for X_2 by conditioning on X_1, and so on.

This result explains why it is called a stationary distribution: once the chain enters this distribution it must remain there.

So if we regard the Markov chain as a map on probability distributions, via the mapping

$$p_j \to \sum_i p_i \, p_{ij}$$

then the stationary distribution is a fixed point for this map. Several immediate questions:

- is there always a stationary distribution?
- if it exists, is the stationary distribution unique?
- does the chain always converge to the stationary distribution?

In general the answer is 'no', but under certain assumptions the answer is yes.

Irreducible and regular

Notation: for a matrix T write $T \geq 0$ if $T_{ij} \geq 0$ for all i, j and $T > 0$ if $T_{ij} > 0$ for all i, j.

Definition 2 *Let P be the transition matrix of a Markov chain.*

(1) *The Markov chain is* irreducible *if for all states i, j there is an integer $n(i, j)$ such that $p_{ij}(n(i, j)) > 0$.*

(2) *The Markov chain is* regular *if there is an integer n such that $P^n > 0$.*

Example 4 *Recall the balls in boxes model:*

$$P = \begin{pmatrix} 0 & 1 & 0 \\ 1/4 & 1/2 & 1/4 \\ 0 & 1 & 0 \end{pmatrix} \tag{14}$$

Since

$$P^2 = \begin{pmatrix} 1/4 & 1/2 & 1/4 \\ 1/8 & 3/4 & 1/8 \\ 1/4 & 1/2 & 1/4 \end{pmatrix} \tag{15}$$

it follows that P is regular.

Example 5 *Define the two-state swapping chain:*

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{16}$$

Then $P^2 = I$ is the identity, hence for all $n \geq 1$

$$P^{2n} = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad P^{2n+1} = P \tag{17}$$

So P is irreducible but not regular.

0.1 Perron-Frobenius Theorem

Let e denote the vector in $\mathbb{R}^n$ with all entries 1, so

$$e = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} = \begin{pmatrix} 1 & \cdots & 1 \end{pmatrix}^T \tag{18}$$

Theorem 2 [Perron-Frobenius] *Suppose P is a regular $n \times n$ transition matrix. Then there is a unique strictly positive vector $w \in \mathbb{R}^n$ such that*

$$w^T P = w^T \tag{19}$$

and such that

$$P^k \to e\, w^T \quad \text{as } k \to \infty \tag{20}$$

Proof of Perron-Frobenius: We show that for all vectors $y \in \mathbb{R}^n$,

$$P^k y \to e\, w^T y \tag{21}$$

which is a positive multiple of the constant vector e. This implies the result.

Suppose first that $P > 0$ so that $p_{ij} > 0$ for all $i, j \in S$. Let $d > 0$ be the smallest entry in P (so $d \leq 1/2$). For any $y \in \mathbb{R}^n$ define

$$m_0 = \min_j \, y_j, \quad M_0 = \max_j \, y_j \tag{22}$$

and

$$m_1 = \min_j \, (Py)_j, \quad M_1 = \max_j \, (Py)_j \tag{23}$$

Consider $(Py)_i = \sum_j p_{ij} y_j$. This is maximized by pairing the smallest entry m_0 of y with the smallest entry d of p_{ij}, and then taking all other entries of y to be M_0. For any i,

$$\begin{aligned}
(Py)_i &= \sum_j p_{ij} y_j \\
&= p_{ik} m_0 + \sum_{j \neq k} p_{ij} y_j && (24) \\
&\leq p_{ik} m_0 + (1 - p_{ik}) M_0 && (25) \\
&\leq d m_0 + (1 - d) M_0 && (26)
\end{aligned}$$

and therefore

$$M_1 \leq d m_0 + (1 - d) M_0$$

By similar reasoning,

$$m_1 = \min_i (Py)_i \geq (1 - d) m_0 + d M_0 \tag{27}$$

Subtracting these bounds gives

$$M_1 - m_1 \leq (1 - 2d)(M_0 - m_0) \tag{28}$$

Now we iterate to give

$$M_k - m_k \leq (1 - 2d)^k \, (M_0 - m_0) \tag{29}$$

where again

$$M_k = \max_i (P^k y)_i, \quad m_k = \min_i (P^k y)_i \tag{30}$$

Furthermore the sequence $\{M_k\}$ is decreasing since

$$M_{k+1} = \max_i (P P^k y)_i = \max_i \sum_j p_{ij} (P^k y)_j \leq M_k \tag{31}$$

and the sequence $\{m_k\}$ is increasing for similar reasons. Therefore both sequences converge as $k \to \infty$, and the difference between them also converges to zero. Hence we conclude that the components of the vector $P^k y$ converge to a constant value, meaning that

$$P^k y \to m\, e \tag{32}$$

for some m.

We can pick out the value of m with the inner product

$$m(e^T e) = e^T \lim_{k\to\infty} P^k y = \lim_{k\to\infty} e^T P^k y \tag{33}$$

Note that for $k \geq 1$,

$$e^T P^k y \geq m_k(e^T e) \geq m_1(e^T e) = \min_i (Py)_i (e^T e)$$

Since P is assumed positive, if $y_i \geq 0$ for all i it follows that $(Py)_i > 0$ for all i, and hence $m > 0$.

Now define

$$w_j = \lim_{k\to\infty} P^k e_j/(e^T e) \tag{34}$$

where e_j is the vector with entry 1 in the j^{th} component, and zero elsewhere. It follows that $w_j > 0$ so w is strictly positive, and

$$P^k \to e w^T \tag{35}$$

By continuity this implies

$$\lim_{k\to\infty} P^k P = e w^T P \tag{36}$$

and hence $w^T P = w^T$. This proves the result in the case where $P > 0$.

Now turn to the case where P is regular. Since P is regular, there exists integer N such that

$$P^N > 0 \tag{37}$$

Hence by the previous result there is a strictly positive $w \in \mathbb{R}^n$ such that

$$P^{kN} \to e w^T \tag{38}$$

as $k \to \infty$, satisfying $w^T P^N = w^T$.

It follows that $P^{N+1} > 0$, and hence there is also a vector v such that

$$P^{k(N+1)} \to e v^T \tag{39}$$

as $k \to \infty$, and $v^T P^{N+1} = v^T$. Considering convergence along the subsequence $kN(N+1)$ it follows that $w = v$, and hence

$$w^T P^{N+1} = v^T P^{N+1} = v^T = w^T = w^T P^N \tag{40}$$

and so

$$w^T P = w^T \tag{41}$$

The subsequence $P^{kN}y$ converges to $ew^T y$ for every y, and we want to show that the full sequence $P^m y$ does the same. For any $\epsilon > 0$ there is $K < \infty$ such that for all $k \geq K$ and all probability vectors y

$$\|(P^{kN} - ew^T)y\| \leq \epsilon \tag{42}$$

Let $m = kN + j$ where $j < N$, then for any probability vector y

$$\|(P^m - ew^T)y\| = \|(P^{kN+j} - ew^T)y\| = \|(P^{kN} - ew^T)P^j y\| \leq \epsilon \tag{43}$$

which proves convergence along the full sequence.

QED

Corollary of Perron-Frobenius Theorem

Note that as a corollary of the Theorem we deduce that the vector w is the unique (up to scalar multiples) solution of the equation

$$w^T P = w^T \tag{44}$$

Also since $v^T e = \sum v_i = 1$ for a probability vector v, it follows that

$$v^T P^n \to w^T \tag{45}$$

for any probability vector v.

Example 6 *Recall the balls in boxes model:*

$$P = \begin{pmatrix} 0 & 1 & 0 \\ 1/4 & 1/2 & 1/4 \\ 0 & 1 & 0 \end{pmatrix} \tag{46}$$

We saw that P is regular. Solving the equation $w^T P = w^T$ yields the solution

$$w^T = (1/6, 2/3, 1/6) \tag{47}$$

Furthermore we can compute

$$P^{10} = \begin{pmatrix} 0.167 & 0.666 & 0.167 \\ 0.1665 & 0.667 & 0.1665 \\ 0.167 & 0.666 & 0.167 \end{pmatrix} \tag{48}$$

showing the rate of convergence.

Meaning of Perron-Frobenius

Concerning the interpretation of the result. Suppose that the distribution of X_0 is

$$P(X_0 = i) = \alpha_i \tag{49}$$

for all $i \in S$. Then

$$\begin{aligned} P(X_k = j) &= \sum_i P(X_k = j | X_0 = i)\, P(X_0 = i) \\ &= \sum_i (P^k)_{ij}\, \alpha_i \\ &= (\alpha^T P^k)_j \end{aligned}$$

where α is the vector with entries α_i. Using our Theorem we deduce that

$$P(X_k = j) \to w_j \tag{50}$$

as $k \to \infty$ for any initial distribution α. Furthermore if $\alpha = w$ then $\alpha^T P^k = w^T P^k = w^T$ and therefore

$$P(X_k = j) = w_j \tag{51}$$

for all k. So w is called the *equilibrium* or *stationary* distribution of the chain. The Theorem says that the state of the chain rapidly forgets its initial distribution and converges to the stationary value.

0.2 Finite and irreducible

Now suppose the chain is irreducible but not regular. Then we get a similar but weaker result.

Theorem 3 *Let P be the transition matrix of an irreducible Markov chain. Then there is a unique strictly positive probability vector w such that*

$$w^T P = w^T \tag{52}$$

Furthermore

$$\frac{1}{n+1}\Big(I + P + P^2 + \cdots + P^n\Big) \to e w^T \tag{53}$$

as $n \to \infty$.

This Theorem allows the following interpretation: for an irreducible chain, w_j is the long-run fraction of time the chain spends in state j.

Proof for finite state irreducible: define

$$Q = \frac{1}{2} I + \frac{1}{2} P \tag{54}$$

Then Q is a transition matrix. Also

$$2^n Q^n = \sum_{k=0}^{n} \binom{n}{k}\; P^k \tag{55}$$

Because the chain is irreducible, for all pairs of states i, j there is an integer $n(i,j)$ such that $(P^{n(i,j)})_{ij} > 0$. Let $n = \max n(i,j)$, then for all i, j we have

$$2^n (Q^n)_{ij} = \sum_{k=0}^{n} \binom{n}{k}\; (P^k)_{ij} \geq \binom{n}{n(i,j)}\; (P^{n(i,j)})_{ij} > 0 \tag{56}$$

and hence Q is regular. Let w be the unique stationary vector for Q then

$$w^T Q = w^T \leftrightarrow w^T P = w^T \tag{57}$$

which shows existence and uniqueness for P.

Let $W = ew^T$ then a calculation shows that for all n

$$\Big(I + P + P^2 + \cdots + P^{n-1}\Big)(I - P + W) = I - P^n + nW \tag{58}$$

Note that $I - P + W$ is invertible: indeed if $y^T(I - P + W) = 0$ then

$$y^T - y^T P + (y^T e)w = 0 \tag{59}$$

Multiply by e on the right and use $Pe = e$ to deduce

$$y^T e - y^T Pe + (y^T e)(w^T e) = (y^T e)(w^T e) = 0 \tag{60}$$

Since $w^T e = 1 > 0$ it follows that $y^T e = 0$ and so $y^T - y^T P = 0$. By uniqueness this means that y is a multiple of w, but then $y^T e = 0$ means that $y = 0$. Therefore $I - P + W$ is invertible, and so

$$I + P + P^2 + \cdots + P^{n-1} = (I - P^n + nW)(I - P + W)^{-1} \tag{61}$$

Now $WP = W = W^2$ hence

$$W(I - P + W) = W \implies W = W(I - P + W)^{-1} \tag{62}$$

Therefore

$$I + P + P^2 + \cdots + P^{n-1} = (I - P^n)(I - P + W)^{-1} + nW \tag{63}$$

and so

$$\frac{1}{n}\Big(I + P + P^2 + \cdots + P^{n-1}\Big) = W + \frac{1}{n}(I - P^n)(I - P + W)^{-1} \tag{64}$$

It remains to show that the norm of the matrix $(I - P^n)(I - P + W)^{-1}$ is bounded as $n \to \infty$, or equivalently that $\|(I - P^n)\|$ is uniformly bounded. This follows from the bound

$$\|P^n z\| \leq \sum_{ij} (P^n)_{ij} |z_j| = \sum_j |z_j| \tag{65}$$

Therefore $\frac{1}{n}(I - P^n)(I - P + W)^{-1} \to 0$ and the result follows,

QED

0.3 Sojourn times

Definition 3 *Consider an irreducible Markov chain.*

(1) starting in state i, m_{ij} is the expected number of steps to visit state j for the first time (by convention $m_{ii} = 0$)

(2) starting in state i, r_i is the expected number of steps for the first return to state i

(3) the fundamental matrix is $Z = (I - P + W)^{-1}$

Theorem 4 *Let w be the stationary distribution of an irreducible finite state Markov chain. Then for all states $i, j \in S$,*

$$r_i = \frac{1}{w_i}, \quad m_{ij} = \frac{z_{jj} - z_{ij}}{w_j} \tag{66}$$

where z_{ij} is the (i, j) entry of the fundamental matrix Z.

Proof: let M be the matrix with entries $M_{ij} = m_{ij}$, let E be the matrix with entries $E_{ij} = 1$, and let D be the diagonal matrix with diagonal entries $D_{ii} = r_i$. For all $i \neq j$,

$$m_{ij} = p_{ij} + \sum_{k \neq j} p_{ik}(m_{kj} + 1) = 1 + \sum_{k \neq j} p_{ik} m_{kj} \tag{67}$$

For all i,

$$r_i = \sum_k p_{ik}(m_{ki} + 1) = 1 + \sum_k p_{ik} m_{ki} \tag{68}$$

Thus for all i, j,

$$M_{ij} = 1 + \sum_{k \neq j} p_{ik} M_{kj} - D_{ij} \tag{69}$$

which can be written as the matrix equation

$$M = E + PM - D \tag{70}$$

Multiplying on the left by w^T and noting that $w^T = w^T P$ gives

$$0 = w^T E - w^T D \tag{71}$$

The i^{th} component of the right side is $1 - w_i r_i$, hence this implies that for all i

$$r_i = \frac{1}{w_i} \tag{72}$$

Recall the definition of the matrix $Z = (I - P + W)^{-1}$, and vector $e = (1, 1, \ldots, 1)^T$. Since $Pe = We = e$ it follows that $(I - P + W)e = e$ and hence $Ze = e$ and $ZE = E = ee^T$. Furthermore $w^T P = w^T W = w^T$ and so similarly $w^T Z = w^T$ and $W = WZ$. Therefore from (**??**),

$$Z(I - P)M = ZE - ZD = E - ZD \tag{73}$$

Since $Z(I - P) = I - ZW = I - W$ this yields

$$M = E - ZD + WM \tag{74}$$

The (i, j) component of this equation is

$$m_{ij} = 1 - z_{ij} r_j + (w^T M)_j \tag{75}$$

Setting $i = j$ gives $0 = 1 - z_{jj} r_j + (w^T M)_j$, hence

$$m_{ij} = (z_{jj} - z_{ij}) r_j = \frac{z_{jj} - z_{ij}}{w_j} \tag{76}$$

$\boxed{\text{QED}}$

0.4 Absorbing chains

Definition 4 *A state i is* absorbing *if $p_{ii} = 1$. A chain is* absorbing *if for every state i there is an absorbing state which is accessible from i. A non-absorbing state in an absorbing chain is called a* transient *state.*

Consider an absorbing chain with r absorbing states and t transient states. Re-order the states so that the transient states come first, then the absorbing states. The transition matrix then has the form

$$P = \begin{pmatrix} Q & R \\ 0 & I \end{pmatrix} \tag{77}$$

where I is the $r \times r$ identity matrix.

Example 7 *For the drunkard's walk, show that*

$$Q = \begin{pmatrix} 0 & 1/2 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 1/2 & 0 \end{pmatrix}, \quad R = \begin{pmatrix} 1/2 & 0 \\ 0 & 0 \\ 0 & 1/2 \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{78}$$

Simple calculations show that for all $n \geq 1$

$$P^n = \begin{pmatrix} Q^n & R_n \\ 0 & I \end{pmatrix} \tag{79}$$

where R_n is a complicated matrix depending on Q and R.

Lemma 2 *As $n \to \infty$,*

$$(Q^n)_{ij} \to 0$$

for all absorbing states i, j.

Proof: for a transient state i, there is an absorbing state k, an integer n_i and $\delta_i > 0$ such that

$$p_{ik}(n_i) = \delta_i > 0 \tag{80}$$

Let $n = \max n_i$, and $\delta = \min \delta_i$, then for any $i \in T$, there is a state $k \in R$ such that

$$p_{ik}(n) \geq \delta \tag{81}$$

Hence for any $i \in T$,

$$\sum_{j \in T} Q^n_{ij} = 1 - \sum_{k \in R} P^n_{ik} = 1 - \sum_{k \in R} p_{ik}(n) \leq 1 - \delta \tag{82}$$

In particular this means that $Q^n_{ij} \leq 1 - \delta$ for all $i, j \in T$. So for all $i \in T$ we get

$$\sum_{j \in T} Q^{2n}_{ij} = \sum_{k \in T} Q^n_{ik} \sum_{j \in T} Q^n_{kj} \leq (1 - \delta) \sum_{k \in T} Q^n_{ik} \leq (1 - \delta)^2 \tag{83}$$

This iterates to give

$$\sum_{j \in T} Q^{kn}_{ij} \to 0 \quad \text{as } k \to \infty \tag{84}$$

for all $i \in T$.

It remains to notice that

$$\sum_{j \in T} Q_{ij}^{m+1} = \sum_{k \in T} Q_{ik}^m \sum_{j \in T} Q_{kj} \leq \sum_{k \in T} Q_{ik}^m \tag{85}$$

and hence the sequence $\{\sum_{k \in T} Q_{ik}^m\}$ is monotone decreasing in m. Therefore

$$\sum_{j \in T} Q_{ij}^k \to 0 \quad \text{as } k \to \infty \tag{86}$$

for all $i \in T$, which proves the result.

QED

Notice what the result says: the probability of remaining in the transient states goes to zero, so eventually the chain must transition to the absorbing states. So the quantities of interest are related to the time (=number of steps) needed until the chain exits the transient states and enters the absorbing states, and the number of visits to other transient states.

Consider the equation

$$x = Qx \tag{87}$$

Applying Q to both sides we deduce that

$$x = Q^2 x \tag{88}$$

and iterating this leads to

$$x = Q^n x \tag{89}$$

for all n. Since $Q^n \to 0$ it follows that $x = 0$. Hence there is no nonzero solution of the equation $x = Qx$ and therefore the matrix $I - Q$ is non-singular and so invertible.

Define the fundamental matrix

$$N = (I - Q)^{-1} \tag{90}$$

Note that

$$(I + Q + Q^2 + \cdots + Q^n)(I - Q) = I - Q^{n+1} \tag{91}$$

and letting $n \to \infty$ we deduce that

$$N = I + Q + Q^2 + \cdots \tag{92}$$

Theorem 5 *Let i, j be transient states. Then*

(1) N_{ij} is the expected number of visits to state j starting from state i (counting initial state if $i = j$).

(2) $\sum_j N_{ij}$ is the expected number of steps of the chain, starting in state i, until it is absorbed.

(3) define the $t \times r$ matrix $B = NR$. Then B_{ik} is the probability that the chain is absorbed in state k, given that it started in state i.

Proof: the chain starts at $X_0 = i$. Given a state $j \in T$, for $k \geq 0$ define indicator random variables as follows:

$$Y^{(k)} = \begin{cases} 1 & \text{if } X_k = j \\ 0 & \text{else} \end{cases} \tag{93}$$

Then for $k \geq 1$

$$\mathbb{E}Y^{(k)} = P(Y^{(k)} = 1) = P(X_k = j) = p_{ij}(k) = (Q^k)_{ij} \tag{94}$$

and for $k = 0$ we get $\mathbb{E}Y^{(0)} = \delta_{ij}$.

Now the number of visits to the state j in the first n steps is $Y^{(0)} + Y^{(1)} + \cdots + Y^{(n)}$. Taking the expected value yields the sum

$$\delta_{ij} + Q_{ij} + (Q^2)_{ij} + \cdots + (Q^n)_{ij} = (I + Q + Q^2 + \cdots + Q^n)_{ij} \tag{95}$$

which converges to N_{ij} as $n \to \infty$. This proves (1).

For (2), note that the sum of visits to all transient states is the total number of steps of the chain before it leaves the transient states. For (3), use $N = \sum Q^n$ to write

$$\begin{aligned} (NR)_{ik} &= \sum_{j \in T} N_{ij} \, R_{jk} \\ &= \sum_{j \in T} \sum_{n=0}^{\infty} (Q^n)_{ij} R_{jk} \\ &= \sum_{n=0}^{\infty} \sum_{j \in T} (Q^n)_{ij} R_{jk} \end{aligned} \tag{96}$$

and note that $\sum_{j \in T} (Q^n)_{ij} R_{jk}$ is the probability that the chain takes n steps to transient states before exiting to the absorbing state k. Since this is the only way that the chain can transition to k in $n+1$ steps, the result follows.

$\boxed{\text{QED}}$

Example 8 *For the drunkard's walk,*

$$Q^{2n+1} = 2^{-n} Q, \quad Q^{2n+2} = 2^{-n} Q^2 \tag{97}$$

and

$$N = \begin{pmatrix} 3/2 & 1 & 1/2 \\ 1 & 2 & 1 \\ 1/2 & 1 & 3/2 \end{pmatrix} \tag{98}$$

Also

$$B = NR = \begin{pmatrix} 3/4 & 1/4 \\ 1/2 & 1/2 \\ 1/4 & 3/4 \end{pmatrix} \tag{99}$$

0.5 Addendum on transient states

There are many interesting problems where transient states are important. We will not say too much about them, but just note that there are generally two questions of interest:

- How long until the chain exits the transient states?
- Which irreducible class will it then enter?

Both questions can be answered in a systematic way by using the *associated absorbing chain* together with its *fundamental matrix*.

Suppose the original chain is decomposed as

$$\Omega = T \cup C_1 \cup C_2 \cup \cdots$$

where T denotes the transient states, and each C_i is a closed irreducible class.

Then the associated absorbing chain has state space

$$\Omega^{abs} = T \cup \{c_1\} \cup \{c_2\} \cup \cdots$$

where T are the same transient states and each closed irreducible class C_i has been replaced by a *single state* c_i.

With respect to this decomposition the transition matrix of the chain on Ω^{abs} is

$$P^{abs} = \begin{pmatrix} Q & R \\ 0 & \mathbb{I} \end{pmatrix}$$

where Q is the original transition matrix between transient states, and

$$R_{tj} = \sum_{a \in C_j} p_{ta}$$

where t is a transient state and the sum runs over all states in the class C_j. Finally $\mathbb{I}$ is the identity matrix on the states $\{c_1\} \cup \{c_2\} \cup \cdots$.

Then the fundamental matrix of the absorbing chain is defined to be

$$N = (\mathbb{I} - Q)^{-1}$$

Lemma 3

- *The matrix element N_{ij} is the expected number of visits of chain to the transient state j starting in the transient state i.*
- *$\sum_j N_{ij}$ is the expected number of steps until the chain exits the transient states, starting in the transient state i.*
- *$\sum_k N_{ik} R_{kj}$ is the probability that the chain will enter the class C_j starting in the transient state i.*

This works well for a small number of transient states, but becomes cumbersome for larger numbers.

0.6 Convergence to the stationary distribution.

An irreducible persistent chain has a unique stationary distribution. It is reasonable to expect that

$$P(X_n = k \,|\, X_0 = i) \to \pi_k$$

as $n \to \infty$. We determine the cases where this holds.

The extra condition needed concerns the period of the chain. For example, the RW has period 2: we saw that $P(X_n = 0 | X_0 = 0) = 0$ unless n is even. This is a special case of periodic behavior.

Definition 5 *The period of the state i is*

$$d(i) = \gcd\{n \,|\, p_{ii}(n) > 0\}$$

The state i is aperiodic if $d(i) = 1$.

Definition 6 *An irreducible, aperiodic, persistent Markov chain is called* ergodic*.*

Theorem 6 *For an ergodic chain,*

$$p_{ij}(n) \to \pi_j = \frac{1}{\mu_j} \tag{100}$$

as $n \to \infty$, for all $i, j \in S$.

0.7 Mixing time for ergodic chain

The ergodic Theorem says that $P(X_n = j) \to \pi_j$ as $n \to \infty$ for every state j. So the chain 'forgets' about its initial state and settles into the stationary distribution.

How long does this process take? This is an interesting question for many applications.

Card shuffling

Persi Diaconis (b. 1945) left school at 14 to travel with a conjurer and learn card tricks. After returning to college he supported himself by playing poker on ships between New York and South America. Diaconis is currently a Professor at Stanford University.

Diaconis famously showed that it takes seven shuffles to randomize a deck of cards. There is a precise statement of this, but roughly it means that starting from an ordered deck, and repeatedly using the 'riffle shuffle', the distance from the uniform distribution (which is the stationary distribution in this case) decreases and gets below 1/2 after 7 shuffles. After this it drops by a factor 1/2 at each subsequent shuffle.

In general convergence to the stationary distribution occurs at an exponential rate (determined by the eigenvalues of the transition matrix).

Rate of convergence

[Seneta]: another way to express the Perron-Frobenius result is to say that for the matrix P, 1 is the largest eigenvalue (in absolute value) and w is the unique eigenvector (up to scalar multiples). Let λ_2 be the second largest eigenvalue of P so that $1 > |\lambda_2| \geq |\lambda_i|$. Let m_2 be the multiplicity of λ_2. Then the following estimate holds: there is $C < \infty$ such that for all $n \geq 1$

$$\|P^n - ew^T\| \leq C\, n^{m_2 - 1}\, |\lambda_2|^n \tag{101}$$

So the convergence $P^n \to ew^T$ is exponential with rate determined by the first spectral gap.

0.8 Time reversible Markov chains

Consider an ergodic chain $\{\dots, X_{n-1}, X_n, \dots\}$ with transition probabilities p_{ij} and stationary distribution π_j. We have

$$p_{ij} = P(X_n = j \mid X_{n-1} = i) \tag{102}$$

Now consider the reversed chain, where we run the sequence backwards: $\{\dots, X_n, X_{n-1}, \dots\}$. The transition matrix is

$$\begin{aligned} q_{ij} &= P(X_{n-1} = j \mid X_n = i) \\ &= \frac{P(X_{n-1} = j, X_n = i)}{P(X_n = i)} \\ &= P(X_n = i \mid X_{n-1} = j) \frac{P(X_{n-1} = j)}{P(X_n = i)} \\ &= p_{ji} \, \frac{P(X_{n-1} = j)}{P(X_n = i)} \end{aligned} \tag{103}$$

Assume that the original chain is in its stationary distribution so that $P(X_n = i) = \pi_i$ for all i, then this is

$$q_{ij} = p_{ji} \, \frac{\pi_j}{\pi_i} \tag{104}$$

Definition 7 *The Markov chain is* reversible *if $q_{ij} = p_{ij}$ for all $i, j \in S$.*

The meaning of this equation is that the chain "looks the same" when it is run backwards in time (in its stationary distribution). So you cannot tell whether a movie of the chain is running backwards or forwards in time. Equivalently, for all $i, j \in S$

$$\pi_i p_{ij} = \pi_j p_{ji} \tag{105}$$

The main advantage of this result is that these equations are much easier to solve than the original defining equations for π. There is a nice result which helps here.

Lemma 4 *Consider an irreducible Markov chain with transition probabilities p_{ij}. Suppose there is a distribution $w_j > 0$ such that for all $i, j \in S$*

$$w_i p_{ij} = w_j p_{ji} \tag{106}$$

Then the chain is time reversible and w_j is the stationary distribution.

So this result says that if you can find a positive solution of the simpler equation then you have solved for the stationary distribution.

Example 9 *A total of m white and m black balls are distributed among two boxes, with m balls in each box. At each step, a ball is randomly selected from each box and the two selected balls are exchanged and put back in the boxes. Let X_n be the number of white balls in the first box after n steps. Show that the chain is time reversible and find the stationary distribution.*

If we can solve the time-reversible equations, we are done. The transition matrix is

$$p_{ij} = P(X_1 = j \,|\, X_0 = i) = \begin{cases} \left(\frac{i}{M}\right)^2 & \textit{for } j = \textit{i-1} \\ 2\left(\frac{i}{M}\frac{M-i}{M}\right) & \textit{for j=i} \\ \left(\frac{M-i}{M}\right)^2 & \textit{for } j = \textit{i+1} \end{cases}$$

Only one time reversible condition needs to be checked:

$$\pi_i p_{i,i+1} = \pi_{i+1} p_{i+1,i}$$

in other words

$$\pi_i \left(\frac{M-i}{M}\right)^2 = \pi_{i+1} \left(\frac{i+1}{M}\right)^2$$

Can check that this is satisfied by

$$\pi_i = \frac{\binom{M}{i}^2}{\binom{2M}{M}}$$

Maybe could have guessed this: this is the probability that a randomly selected set of M balls (drawn from the complete set of $2M$ balls) would contain i white balls and $M - i$ black balls.

The quantity $\pi_i p_{ij}$ has another interpretation: it is the rate of jumps of the chain from state i to state j. More precisely, it is the long-run average rate at which the chain makes the transition between these states:

$$\lim_{n\to\infty} P(X_n = i\,,\, X_{n+1} = j) = \pi_i p_{ij} \tag{107}$$

This often helps to figure out if a chain is reversible.

Example 10 *Random walk on graph.*

Example 11 *Gambler's Ruin.*