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INFORMATION THEORY
MARKOV CHAINS

Throughout, let \mathcal{X} denote a finite set, and refer to its elements as states, hence the terminology state space used sometimes to denote \mathcal{X} . A (square) matrix \mathbf{P} on \mathcal{X} is simply an $|\mathcal{X}| \times |\mathcal{X}|$ array of scalars, one for each ordered pair of states, namely

$$(p_{xy}, x, y \in \mathcal{X}).$$

We shall write $\mathbf{P} = (p_{xy})$ when no confusion arises.

Stochastic matrices

Consider a matrix $\mathbf{P} = (p_{xy})$ on \mathcal{X} . It is said to be a *stochastic matrix* if

$$0 \leq p_{xy} \leq 1, \quad x, y \in \mathcal{X}$$

and

$$\sum_{y \in \mathcal{X}} p_{xy} = 1, \quad x \in \mathcal{X}.$$

Thus, for each x in \mathcal{X} , the row

$$(p_{xy}, y \in \mathcal{X})$$

can be interpreted as a pmf \mathbf{p}_x on \mathcal{X} .

Furthermore, the matrix \mathbf{P} is said to *doubly stochastic* if it is a stochastic matrix such that

$$\sum_{x \in \mathcal{X}} p_{xy} = 1, \quad y \in \mathcal{X}.$$

Powers of \mathbf{P}

The powers \mathbf{P} are defined by

$$\mathbf{P}^0 = \mathbf{I}, \quad \mathbf{P}^{n+1} = \mathbf{P}\mathbf{P}^n = \mathbf{P}^n\mathbf{P}, \quad n = 0, 1, \dots$$

with the identity matrix \mathbf{I} on \mathcal{X} naturally defined by

$$\mathbf{I} = (\delta_{xy}).$$

We shall use the notation

$$P^n = (p_{xy}^{(n)}), \quad n = 0, 1, \dots$$

These definitions are well posed as indicated by the following fact.

Fact 0.1 We have

$$P P^n = P^n P, \quad n = 0, 1, \dots$$

Proof. Easy by induction. ■

Fact 0.2 For every non-negative integers $r, s, t = 0, 1, \dots$, it is always the case that

$$P^{r+s+t} = P^r P^s P^t.$$

Proof. Elementary by associativity of the matrix product. ■

Fact 0.3 If P is a stochastic matrix, then each of the matrices $\{P^n, n = 0, 1, \dots\}$ of P is also a stochastic matrix.

Proof. Easy by induction. ■

Irreducibility

The stochastic matrix P is said to be *irreducible* if for every pair of distinct states x and y in \mathcal{X} there exist positive integers $n(x, y)$ and $n(y, x)$ such that

$$p_{xy}^{(n(x,y))} > 0 \quad \text{and} \quad p_{yx}^{(n(y,x))} > 0.$$

Period

For any non-empty subset $\{n_\alpha, \alpha \in A\}$ of \mathbb{N} , we denote its *greatest common denominator* by

$$\text{g.c.d. } (n_\alpha, \alpha \in A).$$

For each state x in \mathcal{X} we define its *period* $d(x)$ as the integer

$$(1) \quad d(x) = \text{g.c.d. } (n = 1, 2, \dots : p_{xx}^{(n)} > 0)$$

with the convention $d(x) = \infty$ if the set $(n = 1, 2, \dots : p_{xx}^{(n)} > 0)$ is empty. The state x is said to be *periodic* if $d(x) \geq 2$ and *aperiodic* if $d(x) = 1$.

Theorem 0.1 *An irreducible Markov chain P on \mathcal{X} has the property that either all its states are aperiodic or they are all periodic with the same period.*

Proof. Pick two states x and y in \mathcal{X} . The chain P being irreducible, there exist positive integers $n(x, y)$ and $n(y, x)$ such that

$$p_{xy}^{(n(x,y))} > 0 \quad \text{and} \quad p_{yx}^{(n(y,x))} > 0.$$

Therefore,

$$(2) \quad \begin{aligned} p_{yy}^{(n(y,x)+n(x,y))} &= \sum_z p_{yz}^{(n(y,x))} p_{zy}^{(n(x,y))} \\ &\geq p_{yx}^{(n(y,x))} p_{xy}^{(n(x,y))} > 0. \end{aligned}$$

On the other hand, whenever

$$p_{xx}^{(t)} > 0$$

for some $t = 1, 2, \dots$, then

$$(3) \quad \begin{aligned} p_{yy}^{(n(y,x)+t+n(x,y))} &= \sum_z \sum_v p_{yz}^{(n(y,x))} p_{zv}^{(t)} p_{vy}^{(n(x,y))} \\ &\geq p_{yx}^{(n(y,x))} p_{xx}^{(t)} p_{xy}^{(n(x,y))} > 0. \end{aligned}$$

Therefore, $d(y)$ divides both $n(y, x) + n(x, y)$ and $n(y, x) + t + n(x, y)$, hence $d(y)$ divides t since $n(y, x) + t + n(x, y) - (n(y, x) + n(x, y)) = t$. Thus, $d(y)$ divides all the elements of the set $(t = 1, 2, \dots : p_{xx}^{(t)} > 0)$, so that, $d(y)$ divides $d(x)$ (which is defined as the g.c.d of this set). A similar argument shows that $d(x)$ divides $d(y)$, whence $d(x) = d(y)$. ■

Markov chains

Consider a stochastic matrix \mathbf{P} on \mathcal{X} . A collection of \mathcal{X} -valued rvs $\{X_n, n = 0, 1, \dots\}$ (defined on some probability triple $(\Omega, \mathcal{F}, \mathbb{P})$) is said to be a (time-homogeneous) Markov chain with one-step transition probabilities \mathbf{P} if

$$(4) \quad \mathbb{P}[X_0 = x_0, X_1 = x_1, \dots, X_n = x_n] = \mathbb{P}[X_0 = x_0] \cdot \prod_{\ell=0}^{n-1} p_{x_\ell x_{\ell+1}}$$

for each $n = 1, 2, \dots$ and all x_0, x_1, \dots, x_n in \mathcal{X} . The following fact is key to many of the arguments involving Markov chains.

Theorem 0.2 Fix $k = 0, 1, \dots$. Then for each $n = 1, 2, \dots$, we have

$$(5) \quad \mathbb{P}[X_k = x_0, X_{k+1} = x_1, \dots, X_{k+n} = x_n] = \mathbb{P}[X_k = x_0] \cdot \prod_{\ell=0}^{n-1} p_{x_\ell x_{\ell+1}}$$

with arbitrary x_0, x_1, \dots, x_n in \mathcal{X} .

Proof. Fix $k = 1, 2, \dots, n = 1, 2, \dots$ and states x_0, x_1, \dots, x_n in \mathcal{X} . For any collection of states y_0, \dots, y_{k-1} in \mathcal{X} , we have from (4) that

$$(6) \quad \begin{aligned} & \mathbb{P}[X_0 = y_0, \dots, X_{k-1} = y_{k-1}, X_k = x_0, X_{k+1} = x_1, \dots, X_{k+n} = x_n] \\ &= \mathbb{P}[X_0 = y_0] \cdot \prod_{j=0}^{k-2} p_{y_j y_{j+1}} \cdot p_{y_{k-1} x_0} \cdot \prod_{\ell=0}^{n-1} p_{x_\ell x_{\ell+1}}. \end{aligned}$$

Therefore,

$$\begin{aligned} & \mathbb{P}[X_k = x_0, X_{k+1} = x_1, \dots, X_{k+n} = x_n] \\ &= \sum_{y_0, \dots, y_{k-1}} \mathbb{P}[X_0 = y_0, \dots, X_{k-1} = y_{k-1}, X_k = x_0, X_{k+1} = x_1, \dots, X_{k+n} = x_n] \\ &= \sum_{y_0, \dots, y_{k-1}} \mathbb{P}[X_0 = y_0] \cdot \prod_{j=0}^{k-2} p_{y_j y_{j+1}} \cdot p_{y_{k-1} x_0} \cdot \prod_{\ell=0}^{n-1} p_{x_\ell x_{\ell+1}} \\ &= \left(\sum_{y_0, \dots, y_{k-1}} \mathbb{P}[X_0 = y_0] \cdot \prod_{j=0}^{k-2} p_{y_j y_{j+1}} \cdot p_{y_{k-1} x_0} \right) \cdot \prod_{\ell=0}^{n-1} p_{x_\ell x_{\ell+1}} \\ &= \left(\sum_{y_0, \dots, y_{k-1}} \mathbb{P}[X_0 = y_0, \dots, X_{k-1} = y_{k-1}, X_k = x_0] \right) \cdot \prod_{\ell=0}^{n-1} p_{x_\ell x_{\ell+1}} \\ &= \mathbb{P}[X_k = x_0] \cdot \prod_{\ell=0}^{n-1} p_{x_\ell x_{\ell+1}} \end{aligned}$$

as desired. ■

From (4), for all $x_0, x_1, \dots, x_n, x_{n+1}$ in \mathcal{X} , we get both

$$(7) \quad \mathbb{P}[X_0 = x_0, X_1 = x_1, \dots, X_n = x_n] = \mathbb{P}[X_0 = x_0] \cdot \prod_{\ell=0}^{n-1} p_{x_\ell x_{\ell+1}}$$

and

$$(8) \quad \begin{aligned} & \mathbb{P}[X_0 = x_0, X_1 = x_1, \dots, X_n = x_n, X_{n+1} = x_{n+1}] \\ &= \mathbb{P}[X_0 = x_0] \cdot \prod_{\ell=0}^n p_{x_\ell x_{\ell+1}}, \end{aligned}$$

whence

$$(9) \quad \begin{aligned} & \mathbb{P}[X_0 = x_0, X_1 = x_1, \dots, X_n = x_n, X_{n+1} = x_{n+1}] \\ &= \mathbb{P}[X_0 = x_0, X_1 = x_1, \dots, X_n = x_n] \cdot p_{x_n x_{n+1}} \end{aligned}$$

upon direct comparison of (7) and (8).

Building upon these observations, if

$$(10) \quad \mathbb{P}[X_0 = x_0, X_1 = x_1, \dots, X_n = x_n] > 0,$$

it follows that

$$(11) \quad \mathbb{P}[X_{n+1} = x_{n+1} | X_0 = x_0, X_1 = x_1, \dots, X_n = x_n] = p_{x_n x_{n+1}},$$

suggesting the validity of the relation¹

$$(12) \quad \mathbb{P}[X_{n+1} = x_{n+1} | X_n = x_n] = p_{x_n x_{n+1}}.$$

To see that this is indeed the case, we argue as follows: By Theorem 0.2 we get

$$(13) \quad \mathbb{P}[X_n = x_n, X_{n+1} = x_{n+1}] = \mathbb{P}[X_n = x_n] p_{x_n x_{n+1}}.$$

Under (10) we necessarily have

$$(14) \quad \mathbb{P}[X_n = x_n] > 0,$$

¹See discussion below.

and the standard definition

$$(15) \quad \mathbb{P}[X_{n+1} = x_{n+1} | X_n = x_n] = \frac{\mathbb{P}[X_n = x_n, X_{n+1} = x_{n+1}]}{\mathbb{P}[X_n = x_n]}$$

applies. The desired conclusion (12) now follows from (13).

Alternate definition of Markov chains

In most textbooks Markov chains are given a different definition which we now present: A collection of \mathcal{X} -valued rvs $\{X_n, n = 0, 1, \dots\}$ (defined on some probability triple $(\Omega, \mathcal{F}, \mathbb{P})$) is said to be a (time-homogeneous) Markov chain with one-step transition probabilities \mathbf{P} if

$$(16) \quad \begin{aligned} & \mathbb{P}[X_{n+1} = x_{n+1} | X_0 = x_0, X_1 = x_1, \dots, X_n = x_n] \\ & = \mathbb{P}[X_{n+1} = x_{n+1} | X_n = x_n] \end{aligned}$$

for all $x_0, x_1, \dots, x_n, x_{n+1}$ in \mathcal{X} , with

$$(17) \quad \mathbb{P}[X_{n+1} = x_{n+1} | X_n = x_n] = p_{x_n x_{n+1}}.$$

The difficulty with this definition is that the conditional probabilities involved in (16) are well defined only when

$$(18) \quad \mathbb{P}[X_0 = x_0, X_1 = x_1, \dots, X_n = x_n] > 0$$

and

$$(19) \quad \mathbb{P}[X_n = x_n] > 0$$

Obviously, (18) implies (19) but the converse is not true, possibly creating ambiguities with the definitions being inconsistent with each other.²

A possible solution to this difficulty is to read (16)-(17) as stating instead that

$$(20) \quad \mathbb{P}[X_{n+1} = x_{n+1} | X_0 = x_0, X_1 = x_1, \dots, X_n = x_n] = p_{x_n x_{n+1}}$$

with the understanding that if

$$\mathbb{P}[X_0 = x_0, X_1 = x_1, \dots, X_n = x_n] = 0,$$

then the right handside of (20) is taken to be the definition of the conditional probability that $X_{n+1} = x_{n+1}$ given that $X_0 = x_0, X_1 = x_1, \dots, X_n = x_n$. With this definition it is easy to check that both (4) and (12) hold.

²Recall that the conditional probability $\mathbb{P}[A|B]$ is not uniquely defined when $\mathbb{P}[B] = 0$ with each other.

Stationary Markov chains

Consider the (time-homogeneous) Markov chain $\{X_n, n = 0, 1, \dots\}$ with one-step transition probabilities \mathbf{P} . We write

$$\pi_n(x) = \mathbb{P}[X_n = x], \quad \begin{array}{l} x \in \mathcal{X} \\ n = 0, 1, \dots \end{array}$$

and organize these probabilities into a row vector

$$\boldsymbol{\pi}_n = (\pi_n(x), x \in \mathcal{X}).$$

Using the law of total probabilities we get

$$\pi_{n+1}(x) = \sum_y \pi_n(y) p_{yx}, \quad \begin{array}{l} x \in \mathcal{X} \\ n = 0, 1, \dots \end{array}$$

or in vector notation

$$(21) \quad \boldsymbol{\pi}_{n+1} = \boldsymbol{\pi}_n \mathbf{P}, \quad n = 0, 1, \dots$$

Theorem 0.3 Let $\boldsymbol{\mu}$ denote the pmf of the initial condition X_0 . Then, the (time-homogeneous) Markov chain $\{X_n, n = 0, 1, \dots\}$ with one-step transition probabilities \mathbf{P} is stationary if and only if

$$(22) \quad \boldsymbol{\mu} \mathbf{P} = \boldsymbol{\mu}.$$

Any pmf on \mathcal{X} which satisfies (22) is called a *stationary* pmf for \mathbf{P} .

Proof. First, assume that the Markov chain $\{X_n, n = 0, 1, \dots\}$ is stationary. This implies that for each $n = 0, 1, \dots$, the rv X_n has the same distribution as X_0 , i.e., $\boldsymbol{\pi}_n = \boldsymbol{\mu}$. Substituting this information into (21) yields (22).

Conversely, assume that the initial state X_0 is distributed according to a pmf $\boldsymbol{\mu}$ which satisfies the fixed-point equation (22). Using this fact in conjunction with (21) we get that

$$\boldsymbol{\pi}_1 = \boldsymbol{\pi}_0 \mathbf{P} = \boldsymbol{\mu} \mathbf{P} = \boldsymbol{\mu}$$

so that $\boldsymbol{\pi}_0 = \boldsymbol{\mu}$. Iterating we conclude that

$$\boldsymbol{\pi}_n = \boldsymbol{\mu}, \quad n = 0, 1, \dots$$

Fix $k = 0, 1, \dots$ and $n = 1, 2, \dots$. With arbitrary x_0, x_1, \dots, x_n in \mathcal{X} , Theorem 0.2 states that

$$\begin{aligned}
 & \mathbb{P}[X_k = x_0, X_{k+1} = x_1, \dots, X_{k+n} = x_n] \\
 = & \mathbb{P}[X_k = x_0] \cdot \prod_{\ell=0}^{n-1} p_{x_\ell x_{\ell+1}} \\
 = & \mathbb{P}[X_0 = x_0] \cdot \prod_{\ell=0}^{n-1} p_{x_\ell x_{\ell+1}} \\
 (23) \quad = & \mathbb{P}[X_0 = x_0, X_1 = x_1, \dots, X_n = x_n].
 \end{aligned}$$

This establishes the stationarity of the Markov chain. ■

Existence and uniqueness of stationary pmfs

The stationary pmf is *not* unique if \mathbf{P} is *not* irreducible: For instance, with $\mathcal{X} = \{0, 1\}$ and $\mathbf{P} = \mathbf{I}$, every pmf on \mathcal{X} is a stationary pmf.

More generally, partition \mathcal{X} into two non-empty subsets \mathcal{X}_1 and \mathcal{X}_2 so that $\mathcal{X} = \mathcal{X}_1 \cup \mathcal{X}_2$. Assume the stochastic matrix \mathbf{P} on \mathcal{X} to be of the form

$$(24) \quad \mathbf{P} = \begin{pmatrix} \mathbf{P}_1 & \mathbf{O}_{12} \\ \mathbf{O}_{21} & \mathbf{P}_2 \end{pmatrix}$$

with \mathbf{P}_1 and \mathbf{P}_2 stochastic matrices on \mathcal{X}_1 and \mathcal{X}_2 , respectively. Here \mathbf{O}_{11} and \mathbf{O}_{21} are matrices with all zero entries of the appropriate dimensions. Assume now that $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$ are stationary pmfs for \mathbf{P}_1 and \mathbf{P}_2 , respectively. For each λ in $(0, 1)$, the pmf $\boldsymbol{\mu}_\lambda$ on \mathcal{X} defined by

$$\boldsymbol{\mu}_\lambda = (\lambda \boldsymbol{\mu}_1, (1 - \lambda) \boldsymbol{\mu}_2)$$

is stationary pmf for \mathbf{P} .

Limit theorems for Markov chains

Several limit results are available under certain conditions. The strongest such results guarantee the convergence

$$(25) \quad \lim_{n \rightarrow \infty} \pi_n(x) = \pi(x), \quad x \in \mathcal{X}$$

for some pmf π on \mathcal{X} , or in vector notation

$$(26) \quad \lim_{n \rightarrow \infty} \pi_n = \pi.$$

Sometimes it is only possible to show that

$$(27) \quad \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=0}^{n-1} \pi_k(x) = \pi(x), \quad x \in \mathcal{X}$$

for some pmf π on \mathcal{X} , or in vector notation

$$(28) \quad \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=0}^{n-1} \pi_k = \pi.$$

Obviously (25)-(26) implies (27)-(28) since usual convergence implies Cesaro convergence.

Before giving conditions for either (25)-(26) or (27)-(28) to hold, we make a couple of comments as to the identify of the limit pmf π appearing there.

If (25)-(26) takes place, then letting n go to infinity in (21) we conclude that

$$(29) \quad \begin{aligned} \lim_{n \rightarrow \infty} \pi_{n+1} &= \lim_{n \rightarrow \infty} (\pi_n P) \\ &= \left(\lim_{n \rightarrow \infty} \pi_n \right) P \end{aligned}$$

since finite summation permute with limits. Thus, in the limit

$$(30) \quad \pi = \pi P$$

and π is necessarily a stationary pmf for P .

In a similar vein, for each $n = 1, 2, \dots$, we find

$$(31) \quad \begin{aligned} &\frac{1}{n+1} \sum_{k=0}^n \pi_k \\ &\frac{1}{n+1} \left(\pi_0 + \sum_{k=1}^n \pi_{k-1} P \right) \\ &= \frac{1}{n+1} \pi_0 + \frac{n}{n+1} \cdot \left(\frac{1}{n} \sum_{k=1}^n \pi_{k-1} \right) P. \end{aligned}$$

Letting n go to infinity and assuming that (27)-(28) holds, we readily conclude that the limit π in (27)-(28) again satisfies (30), and π is necessarily a stationary pmf for \mathbf{P} .

The case

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

with $\mathcal{X} = \{0, 1\}$ is quite instructive. Obviously \mathbf{P} is irreducible and periodic with all states having period two. It is also easy to see that for any pmf π on the initial state X_0 , we have

$$\mathbb{P}[X_n = 1] = \begin{cases} \mathbb{P}[X_0 = 1] = \pi(1) & \text{if } n \text{ odd} \\ \mathbb{P}[X_0 = 0] = 1 - \pi(1) & \text{if } n \text{ even} \end{cases}$$

It is now plain that (25)-(26) does not hold unless $\pi(1) = \pi(0) = \frac{1}{2}$, i.e., the uniform pmf on \mathcal{X} . Observe also that (27)-(28) always holds in this case with π uniform on \mathcal{X} . Thus, irreducibility is not sufficient by itself to ensure (25)-(26). Failure to have convergence can be traced to periodicity.

Theorem 0.4 *If the Markov chain is irreducible and aperiodic, then there exists a unique stationary pmf μ for \mathbf{P} and (25)-(26) always holds with limit μ .*

Theorem 0.5 *If the Markov chain is irreducible (and possibly periodic), then there exists a unique stationary pmf μ for \mathbf{P} and (27)-(28) always holds with limit μ .*

Consider the case

$$(32) \quad \mathbf{P} = \begin{pmatrix} a & 1-a \\ 1-b & b \end{pmatrix} \quad \text{with } 0 \leq a, b \leq 1$$

The cases $a = b = 1$ and $a = b = 0$ have already been discussed. It is straightforward to check that (22) takes the form

$$(33) \quad \begin{aligned} \mu(0) &= a\mu(0) + (1-b)\mu(1) \\ \mu(1) &= (1-a)\mu(0) + b\mu(1) \end{aligned}$$

This reduces to

$$(1-a)\mu(0) = (1-b)\mu(1)$$

and the constraint $\mu(0) + \mu(1) = 1$ yields

$$\mu(0) = \frac{1 - a}{2 - (a + b)} \quad \text{and} \quad \mu(1) = \frac{1 - b}{2 - (a + b)}$$

provided $a + b < 2$, in which case (22) has a unique solution! The case $a + b = 2$ is equivalent to $a = b = 1$, for which there are infinitely solutions as we have seen earlier.
