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The Combinatorial Structure of Non-Homogeneous Markov Chains

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1. The Combinatorial Structure of Homogeneous Chains

The classical theory of continuous-parameter Markov chains, as described for instance in [1], assumes that the transition probabilities

$$\mathbf{P}\{X(t)=j \mid X(s)=i\} \qquad (s<t), \tag{1}$$

where i and j run over the countable state space I, are functions

$$p_{ij}(t-s) \tag{2}$$

of $(t-s)$ alone. In this theory one important result is the *Lévy dichotomy*, proved in full generality by Austin and Ornstein (see [1]), which asserts that if the functions $p_{ij}(\cdot)$ are Lebesgue measurable, then each of them is either always or never zero. Thus the relation R on I defined by

$$R=\{(i,j);\, p_{ij}(t)>0\} \tag{3}$$

is independent of $t>0$.

A consequence of this result is that, if $(i,j)\in R$ and $(j,k)\in R$, then for $s,t>0$,

$$p_{ik}(s+t)\geqq p_{ij}(s)\, p_{jk}(t)>0,$$

so that $(i,k)\in R$. Thus R is necessarily a transitive relation. Moreover, if the chain is standard, $(i,i)\in R$ for all $i\in I$, so that R is reflexive.

Conversely, suppose that R is any reflexive transitive relation on the countable set I. Then there exist standard chains on I which satisfy (3); consider for example a q-bounded chain whose infinitesimal generator (q_{ij}) satisfies

$$q_{ij}>0 \Leftrightarrow i\neq j, \quad (i,j)\in R. \tag{4}$$

Thus the problem of characterising the relation (3) for *homogeneous* chains (those for which the conditional probability (1) takes the form (2)) has a very simple solution; the possible relations R are exactly the reflexive transitive relations on I.

This fact has consequences for the embedding problem [3]. Thus, if $(p_{ij};\, i,j\in I)$ is a stochastic matrix, and if there exist $\alpha,\beta,\gamma\in I$ with

$$p_{\alpha\beta}>0, \qquad p_{\beta\gamma}>0, \qquad p_{\alpha\gamma}=0,$$

then there is no homogeneous chain whose transition probabilities satisfy

$$p_{ij}(t)=p_{ij}, \qquad (i,j\in I),$$

for some $t>0$.

The purpose of this paper is to investigate the corresponding problem for non-homogeneous Markov chains. Our main result is Theorem 3, which provides a complete solution when the state space I is finite. The methods depend heavily on the finiteness of I, and a generalisation to infinite state spaces would require new techniques.

2. Non-Homogeneous Markov Chains

Let I be a finite set, and $[a, b]$ a compact, non-degenerate interval. The transition probabilities of a non-homogeneous Markov chain with state space I and parameter space $[a, b]$ are functions

$$p_{ij}(s, t) \quad (a \leqq s \leqq t \leqq b) \tag{5}$$

which satisfy

$$p_{ij}(s, t) \geqq 0, \tag{6}$$

$$\sum_{j \in I} p_{ij}(s, t) = 1, \tag{7}$$

$$p_{ij}(t, t) = \delta_{ij}, \tag{8}$$

$$p_{ij}(s, u) = \sum_{k \in I} p_{ik}(s, t)\, p_{kj}(t, u), \tag{9}$$

for $a \leqq s \leqq t \leqq u \leqq b$. To avoid pathological examples, it will be supposed also that

$$p_{ij}(s, t) \textit{ is separately continuous in } s \textit{ and in } t. \tag{10}$$

An example of an array (p_{ij}) satisfying (6)–(10) is given by

$$p_{ij}(s, t) = p_{ij}(t - s), \tag{11}$$

where $p_{ij}(\cdot)$ are the transition probabilities of a standard homogeneous chain. More generally, let $a = x_0 < x_1 < x_2 < \cdots < x_n = b$ be a dissection of $[a, b]$, and for each α in $1 \leqq \alpha \leqq n$ let $p_{ij}^{(\alpha)}(\cdot)$ be the transition probabilities of a standard homogeneous chain. Define the matrix

$$P(s, t) = (p_{ij}(s, t);\, i, j \in I)$$

by

$$P(s, t) = P^{(\alpha)}(x_\alpha - s) \prod_{\gamma = \alpha + 1}^{\beta - 1} P^{(\gamma)}(x_\gamma - x_{\gamma - 1})\, P^{(\beta)}(t - x_{\beta - 1}), \tag{12}$$

where $x_{\alpha-1} \leqq s \leqq x_\alpha$, $x_{\beta-1} \leqq t \leqq x_\beta$. Then it is easily checked that (6)–(10) are satisfied.

Our problem is to establish the properties of the relation $R(s, t)$ defined on I by

$$R(s, t) = \{(i, j);\, p_{ij}(s, t) > 0\}. \tag{13}$$

In the rest of the paper it will be assumed that I *is finite and that the functions* (5) *satisfy* (6), (8), (9) *and* (10). Eq. (7) is for our purposes irrelevant and will not be assumed. The identity relation on I will be denoted by Δ:

$$\Delta = \{(i, i);\, i \in I\}. \tag{14}$$

Theorem 1. *The relation $R(s,t)$ is reflexive, and $R(t,t)=\Delta$. If $s<t<u<v$, then*

$$R(t,u)\subseteq R(s,v). \tag{15}$$

Proof. That $R(t,t)=\Delta$ follows from (8). For any $i\in I$, $t\in[a,b)$, (10) implies that

$$p_{ii}(t,t+h)>0$$

for all sufficiently small $h>0$, and for $t\in(a,b]$ that

$$p_{ii}(t-h,t)>0$$

for all sufficiently small $h>0$. Since I is finite and

$$p_{ii}(t-h_1,t+h_2)\geqq p_{ii}(t-h_1,t)\,p_{ii}(t,t+h_2),$$

it follows that, for each $t\in[a,b]$, there exists $\delta(t)>0$ such that

$$p_{ii}(s,u)>0$$

whenever $i\in I$ and

$$t-\delta(t)\leqq s\leqq t\leqq u\leqq t+\delta(t).$$

The intervals

$$I(t)=\big(t-\delta(t),t+\delta(t)\big), \quad (a<t<b)$$

cover $[a+\delta(a),b-\delta(b)]$ and hence admit a finite subcover. If $\{I(y_r);\,r=1,2,\dots,n\}$ is a minimal subcover, with $y_1<y_2<\cdots<y_n$, it is easy to see that there exist $x_0,x_1,\dots,x_n$ with

$$a<x_0<y_1<x_1<y_2<\cdots<y_n<x_n<b$$

and

$$y_r-\delta(y_r)\leqq x_{r-1}\leqq y_r\leqq x_r\leqq y_r+\delta(y_r),$$

$$x_0\leqq a+\delta(a), \quad x_n\geqq b-\delta(b).$$

Thus

$$p_{ii}(x_{r-1},x_r)>0,$$

so that

$$p_{ii}(a,b)\geqq p_{ii}(a,x_0)\prod_{r=1}^{n} p_{ii}(x_{r-1},x_r)\,p_{ii}(x_n,b)>0.$$

This implies that $R(a,b)$ is reflexive, and the same arguments apply to the smaller interval (s,t) to show that $R(s,t)$ is also reflexive whenever $a\leqq s\leqq t\leqq b$.

If $s\leqq t\leqq u\leqq v$ and $(i,j)\in R(t,u)$, then

$$p_{ij}(s,v)\geqq p_{ii}(s,t)\,p_{ij}(t,u)\,p_{jj}(u,v)>0,$$

so that $(i,j)\in R(s,v)$, establishing (15) and completing the proof.

3. Some Combinatorial Theory

If R_1 and R_2 are reflexive relations on the set I, another reflexive relation R_1R_2 may be defined by

$$R_1R_2=\{(i,j);\,(i,k)\in R_1,\,(k,j)\in R_2 \text{ for some } k\in I\}. \tag{16}$$

With this definition of "multiplication" the reflexive relations on I form a semigroup (non-commutative if $|I| \geqq 3$) with identity Δ. Clearly

$$R_1 \subseteq R_1', R_2 \subseteq R_2' \Rightarrow R_1 R_2 \subseteq R_1' R_2', \tag{17}$$

and in particular, since $\Delta \subseteq R$ for any reflexive relation R,

$$R_1 \subseteq R_1 R_2, \quad R_2 \subseteq R_1 R_2. \tag{18}$$

This construction is particularly apposite for the present problem, since it follows from (9) that, whenever $s \leqq t \leqq u$,

$$R(s, u) = R(s, t) R(t, u). \tag{19}$$

If R is any reflexive relation on I, a new relation $\tau(R)$ on I may be defined by

$$\tau(R) = \{(i, j); (j, k) \in R \Rightarrow (i, k) \in R\}. \tag{20}$$

Thus $(i, j) \in \tau(R)$ unless there exists $k \in I$ with $(j, k) \in R$, $(i, k) \notin R$.

Theorem 2. *The relation $\tau(R)$ is reflexive and transitive, and satisfies*

$$\tau(R) \subseteq R \tag{21}$$

(with equality if and only if R is transitive) and

$$R = \tau(R) R. \tag{22}$$

Proof. Clearly $(i, i) \in \tau(R)$, so that $\tau(R)$ is reflexive. If $(i, j) \in \tau(R)$ and $(j, l) \in \tau(R)$, then

$$(l, k) \in R \Rightarrow (j, k) \in R \Rightarrow (i, k) \in R,$$

showing that $(i, l) \in \tau(R)$, so that $\tau(R)$ is transitive.

If $(i, j) \in \tau(R)$, then $(j, j) \in R \Rightarrow (i, j) \in R$, proving (21). If equality holds in (21), then $R = \tau(R)$ is transitive. Conversely, if R is transitive,

$$(i, j) \in R \Rightarrow \{(j, k) \in R \Rightarrow (i, k) \in R\} \Rightarrow (i, j) \in \tau(R),$$

so that $\tau(R) = R$.

By (18), $R \subseteq \tau(R) R$. To establish the opposite inclusion, suppose that

$$(i, j) \in \tau(R) R,$$

so that there exists $k \in I$ with

$$(i, k) \in \tau(R), \quad (k, j) \in R.$$

The definition of $\tau(R)$ shows that $(i, j) \in R$, and (22) is proved.

4. The Main Theorem

Theorem 3. *The relation $R(a, b)$ may be expressed as a finite product*

$$R(a, b) = T_1 T_2 \ldots T_n, \tag{23}$$

where each T_r is reflexive and transitive.

Proof. If $R(a,b)=\Delta$ the result is trivial, since Δ is transitive. Suppose therefore that $R(a,b)=R\supset\Delta$, and define

$$x=\sup\{t;\,R(t,b)=R\}.$$

We first prove that

$$R(x,b)\subset R. \tag{24}$$

By (15), $R(x,b)\subseteq R$, so that if (24) is false, $R(x,b)=R$ and therefore $x<b$. If this is so, then by continuity there exists ξ in $x<\xi<b$ such that

$$p_{ij}(\xi,b)>0$$

for all pairs (i,j) such that

$$p_{ij}(x,b)>0.$$

Hence $R(x,b)\subseteq R(\xi,b)$ and, for $a\leqq t<\xi$,

$$R=R(x,b)\subseteq R(\xi,b)\subseteq R(t,b)\subseteq R(a,b)=R,$$

so that

$$R(t,b)=R \qquad (a\leqq t<\xi),$$

which contradicts the definition of x. The contradiction proves (24), which also shows that $x>a$.

Now suppose, if possible, that

$$(i,j)\in R, \qquad (i,j)\notin\tau(R).$$

Then there exists $k\in I$ with

$$(j,k)\in R, \qquad (i,k)\notin R.$$

Take $t<x$, so that

$$(j,k)\in R=R(t,b).$$

Then $(i,j)\in R(a,t)$ would imply

$$(i,k)\in R(a,t)\,R(t,b)=R$$

contrary to hypothesis, and so we must have

$$p_{ij}(a,t)=0.$$

This holds for all $t<x$, so that by continuity

$$p_{ij}(a,x)=0.$$

Hence

$$(i,j)\in R, \qquad (i,j)\notin\tau(R)\Rightarrow(i,j)\notin R(a,x),$$

and since $R(a,x)\subseteq R$ it follows that

$$R(a,x)\subseteq\tau(R). \tag{25}$$

Therefore, by (22),

$$R=R(a,b)=R(a,x)\,R(x,b)\subseteq\tau(R)\,R(x,b)\subseteq\tau(R)\,R=R,$$

showing that

$$R(a,b)=\tau\big(R(a,b)\big)\,R(x,b). \tag{26}$$

We now proceed by induction. Write $x_0=a$, $x_1=x$ and note that, unless $R(x,b)=\Delta$, the argument just described applies to $R(x_1,b)$ to give

$$x_2=\sup\{t;\ R(t,b)=R(x_1,b)\},$$
$$R(x_2,b)\subset R(x_1,b),$$
$$R(x_1,b)=\tau(R(x_1,b))\,R(x_2,b).$$

Continuing, we have a sequence

$$a=x_0<x_1<x_2<\cdots$$

with

$$R(x_{m+1},b)\subset R(x_m,b), \tag{27}$$
$$R(x_m,b)=\tau(R(x_m,b))\,R(x_{m+1},b). \tag{28}$$

The process can only terminate when $R(x_n,b)=\Delta$, and this must be reached after a finite number of steps because of (27) and the finiteness of I. Then (23) follows from (28) on writing

$$T_m=\tau(R(x_{m-1},b)),$$

and the proof is complete.

The conclusion of the theorem is the best possible, since if T_m is any reflexive transitive relation, it can be realised in terms of a standard homogeneous chain. Sticking together the chains realising $T_1, T_2, \ldots, T_m$ in the manner described by (12), we have a non-homogeneous chain satisfying (23). In other words, let us call a relation R *embeddable* if there is a non-homogeneous chain with $R(s,t)=R$ for some $s\leqq t$. Then R is embeddable if and only if it is expressible as a finite product of reflexive transitive relations.

It is possible to give a crude upper bound for n in terms of the number $N=|I|$ of elements of I. Thus (27) shows that

$$|R(x_{m+1},b)|\leqq|R(x_m,b)|-1,$$

so that

$$N=|\Delta|=|R(x_n,b)|\leqq|R(x_0,b)|-n\leqq N^2-n,$$

and therefore

$$n\leqq N^2-N. \tag{29}$$

5. An Algorithm

Theorem 3 reduces the problem of deciding whether a given pattern of positive elements can arise in the transition matrix of a non-homogeneous chain to the combinatorial problem of deciding whether a given relation can be written as a finite product of reflexive transitive relations. The proof of the theorem also suggests an algorithm for solving this combinatorial problem.

If R and R_1 are reflexive relations on the finite set I, call R_1 a *child* of R if

$$R_1\subset R, \qquad R=\tau(R)\,R_1. \tag{30}$$

Lemma. *A reflexive relation R has at least one child if and only if $\tau(R)\neq\Delta$.*

Proof. If $\tau(R)=\Delta$, then the conditions (30) become mutually contradictory:

$$R_1 \subset R, \quad R=R_1.$$

Suppose therefore that $\tau(R)\supset\Delta$, and set

$$S=\{R\smallsetminus\tau(R)\}\cup\Delta.$$

Then S is reflexive, $S\subset R$ and, since $S\subseteq\tau(R)\,S$ and $\tau(R)\subseteq\tau(R)\,S$,

$$R=S\cup\tau(R)\subseteq\tau(R)\,S\subseteq\tau(R)\,R=R.$$

Hence S is a child of R (and so likewise is every relation R_1 with $S\subseteq R_1\subset R$).

Children of a reflexive relation R may themselves have children, and so on, so that a family tree may be built up for R. Since a child has fewer elements than its parent, such a tree has at most $|R|-N$ generations.

Theorem 4. *A reflexive relation R is embeddable if and only if it has a transitive descendant.*

Proof. If R has a transitive descendant T, there is a sequence

$$R=R_0, R_1, R_2, \ldots, R_{n-1}=T$$

in which R_m is a child of R_{m-1}. Writing $T_m=\tau(R_{m-1})$ so that $T_n=T$, we have

$$R_{m-1}=T_m R_m,$$

whence $R=T_1 T_2 \ldots T_n$.

Conversely, if R is embeddable, then there is a non-homogeneous chain with $R(a,b)=R$. By (27) and (28), $R(x_{m+1},b)$ is a child of $R(x_m,b)$, so that $\Delta=R(x_n,b)$ is a descendant of $R(x_0,b)=R$. Hence R has the transitive descendant Δ, and the proof is complete.

Corollary. *A relation R with*

$$R\supset\Delta, \quad \tau(R)=\Delta \tag{31}$$

is not embeddable.

As a simple example of the use of this result, let $I=\{1,2,3,4\}$,

$$P=\begin{pmatrix} \frac{2}{3} & 0 & 0 & \frac{1}{3} \\ 0 & \frac{2}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & \frac{2}{3} & 0 \\ 0 & \frac{1}{3} & 0 & \frac{2}{3} \end{pmatrix} \tag{32}$$

and $R=\{(i,j);\, p_{ij}>0\}$. Since $\tau(R)=\Delta$, R is not embeddable, and so P is not embeddable as $P(s,t)$ for a Markov transition function satisfying (6)–(10). However,

$$\prod_i p_{ii}>\det P>0,$$

so that (32) is a counter-example to the conjecture at the end of § 6 of Goodman's paper [2].

6. A Structure Theory

Theorem 3 shows that the relation $R(a,b)$ is expressible as a finite product of reflexive transitive relations T_r, but it asserts no direct significance for the T_r. Nor does it give any information about the structure of the family of relations $R(s,t)$ $(a \leqq s \leqq t \leqq b)$, beyond the obvious fact that each is embeddable. The next result shows that (roughly speaking) $R(s,t)$ is transitive when the interval (s,t) is small.

Theorem 5. *For each $t \in (a,b]$ there is a reflexive transitive relation $\Gamma_-(t)$ on I such that*

$$R(t-h,t)=\Gamma_-(t) \tag{33}$$

for all sufficiently small $h>0$. For each $t \in [a,b)$, there is a reflexive transitive relation $\Gamma_+(t)$ such that

$$R(t,t+h)=\Gamma_+(t) \tag{34}$$

for all sufficiently small $h>0$.

Proof. Using the notation of the proof of Theorem 3, we distinguish two cases:

(i) If $x_n<b$, then $R(b-h,b)=\Delta$ whenever $0<h<b-x_n$, so that (33) holds when $t=b$ with $\Gamma_-(b)=\Delta$.

(ii) If $x_n=b$, then the definition of x_n implies that, whenever $0<h<b-x_{n-1}$,

$$\begin{aligned} R(b-h,b) &= R(x_{n-1},b) \\ &= \tau\big(R(x_{n-1},b)\big)\, R(x_n,b) \\ &= \tau\big(R(x_{n-1},b)\big), \end{aligned}$$

so that (33) holds when $t=b$ with

$$\Gamma_-(b)=\tau\big(R(x_{n-1},b)\big),$$

which is reflexive and transitive.

Hence we have proved the first part when $t=b$, and applying the same arguments to the chain on $[a,t]$ proves it for all $t \in (a,b]$.

If the matrices $P(s,t)=\big(p_{ij}(s,t)\big)$ satisfy (6), (8), (9) and (10), then so do the matrices

$$P^*(s,t)=P(a+b-t,\,a+b-s)^T, \tag{35}$$

A^T denoting the transpose of the matrix A. Applying the first part of the theorem to this dual family yields the second part of the theorem.

The relations $\Gamma_+(\cdot)$ and $\Gamma_-(\cdot)$ describe the local structure of $R(\cdot,\cdot)$, and might be called the *germs* of the family of relations $R(s,t)$. They contain enough information to allow the $R(s,t)$ to be reconstructed.

Theorem 6. *For any dissection*

$$D\colon s=x_0<x_1<x_2<\cdots<x_n=t \tag{36}$$

of $[s,t]$, define a relation

$$R_D=\Gamma_+(x_0)\prod_{r=1}^{n-1}\{\Gamma_-(x_r)\,\Gamma_+(x_r)\}\,\Gamma_-(x_n). \tag{37}$$

Then, if D_2 is a refinement of D_1,

$$R_{D_1} \subseteq R_{D_2} \subseteq R(s,t), \tag{38}$$

and there exists a dissection D with

$$R_D = R(s,t). \tag{39}$$

Proof. It follows from Theorem 5 and (15) that

$$R(u,v) \supseteq \Gamma_+(u), \qquad R(u,v) \supseteq \Gamma_-(v),$$

and hence that, if $y_r = \frac{1}{2}(x_{r-1} + x_r)$,

$$\begin{aligned} R(s,t) &= R(x_0, y_1) \prod_{r=1}^{n-1} \{R(y_r, x_r) R(x_r, y_{r+1})\} R(y_n, x_n) \\ &\supseteq \Gamma_+(x_0) \prod_{r=1}^{n-1} \{\Gamma_-(x_r) \Gamma_+(x_r)\} \Gamma_-(x_n) \\ &= R_D . \end{aligned}$$

If D_2 is a refinement of D_1, then repeated application of (18) shows that $R_{D_1} \subseteq R_{D_2}$, so that (38) is proved.

Theorem 5 shows that, for each $x \in [a,b]$, there exists $\delta(x) > 0$ such that

$$\begin{aligned} R(x-h, x) &= \Gamma_-(x), \qquad 0 < h \leqq \min(\delta(x), x-a), \\ R(x, x+h) &= \Gamma_+(x), \qquad 0 < h \leqq \min(\delta(x), b-x). \end{aligned}$$

As in the proof of Theorem 1, we can find points

$$s = x_0 < \xi_1 < x_1 < \xi_2 < \cdots < \xi_n < x_n = t,$$

with

$$x_r - \delta(x_r) \leqq \xi_r < x_r < \xi_{r+1} \leqq x_r + \delta(x_r).$$

Then

$$R(\xi_r, x_r) = \Gamma_-(x_r), \qquad R(x_r, \xi_{r+1}) = \Gamma_+(x_r),$$

so that

$$R(s,t) = R(s, \xi_1) \prod_{r=1}^{n-1} \{R(\xi_r, x_r) R(s_r, \xi_{r+1})\} R(\xi_n, t) = R_D$$

if D is the dissection (36). Hence the theorem is proved.

If the dissections D of $[s,t]$ are ordered by refinement and relations on I by inclusion, then (38) and (39) assert that the map $D \mapsto R_D$ is monotone, and that

$$R(s,t) = \sup_D R_D, \tag{40}$$

the supremum being attained. Thus (40) expresses $R(s,t)$ explicitly in terms of the germs at points in $[s,t]$. It should be noted, however, that there is in general no simple relation between the dissections which attain the suprema in (40) for different intervals $[s,t]$.

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