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A CHARACTERIZATION OF REVERSIBLE MARKOV CHAINS BY A ROTATIONAL REPRESENTATION

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Let $P = (p_{ij})$, $i, j = 1, 2, \ldots, n$ be the matrix of a recurrent Markov chain with stationary vector $v > 0$ and let $R = (r_{ij})$, $i, j = 1, 2, \ldots, n$ be a matrix, where $r_{ij} = v_i p_{ij}$. If R is a symmetric matrix, we improve Alpern's rotational representation of P. By this representation we characterize the reversible Markov chains.

1. Introduction. Let $P = (p_{ij})$, $i, j = 1, 2, \ldots, n$ be a stochastic recurrent matrix with stationary vector $(v_1, \ldots, v_n)$. Let m denote Lebesgue measure on $[0, 1)$ and let $f_t(x) = (x + t)(\mathrm{mod}\, 1)$ be the shift transformation on $[0, 1)$. Let $S = (S_i,\ i = 1, 2, \ldots, n)$ be a partition of the unit interval. We say that S has type L if every S_i can be represented as a union of at most L intervals. We say that (t, S) is a rotational representation of P if

$$p_{ij} = \big(m\big(f_t(S_i) \cap S_j\big)\big)/m(S_i) \quad \text{with } m(S_i) = v_i,\ i = 1, 2, \ldots, n.$$

Cohen (1981) proved that every 2×2 recurrent matrix has a rotational representation of type 1 and conjectured that every $n \times n$ irreducible stochastic matrix has a rotational representation where S has type n − 1. Alpern (1983) showed that Cohen's conjecture was false. Haigh (1985) gave a type 2 representation for 3×3 recurrent matrices and Alpern gave a representation for $n \times n$ recurrent matrices. The type of this representation is very far from Cohen's conjecture.

Cohen suggested such a representation by looking at 2×2 recurrent matrices. These matrices have the property of being reversible matrices. We say that P is reversible if

$$p_{ij} = (v_j p_{ji})/v_i \qquad i, j = 1, \ldots, n.$$

Define $R = (r_{ij})$, $i, j = 1, \ldots, n$, where $r_{ij} = v_i p_{ij}$. P is a reversible matrix iff R is a symmetric matrix.

We will show that every $n \times n$ reversible matrix has a rotational representation $(\frac{1}{2}, S)$ of type $[n/2] + 1$, so this representation improves Cohen's conjecture if $n > 4$. We also use this representation to characterize reversible matrices.

2. Rotational representation of reversible recurrent matrices. The construction given by Alpern (1983) is based on the decomposition of the

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matrix R into cycles and on the assignment of labels to each subinterval of a partition. The type of the partition depends on the order of the cycles and on the way the labels are assigned to each subinterval. If R is a symmetric matrix, then it is a convex combination of n cycle matrices of length one and $n(n-1)/2$ cycle matrices of length two, so the rotation can be taken to be π, that is $t = \frac{1}{2}$. In this case the cycles and the labels can be reordered to get the labels grouped at least in pairs except, perhaps, one of them. As two or more contiguous subintervals with the same label can be merged into one, we have less intervals than labels, therefore the type of the partition decreases.

The following lemma proves that such ordering and labeling can be found.

LEMMA 1. *Let $E = E(n)$ be the set of $N = n + n(n-1)/2$ unordered pairs (i, j) with i, j in $\{1, \dots, n\}$. Then the elements of E may be ordered and labeled as $(a(k), b(k))$, $k = 1, \dots, N$, so that in the circular arrangement $a(1), a(2), \dots, a(N), b(1), \dots, b(N)$ [i.e., with $a(1)$ adjacent to $b(N)$] the $n+1$ occurrences of each label i form at most $[n/2] + 1$ contiguous sets.*

PROOF. First assume n is odd. Let G be the graph with vertices $1, \dots, n$ and edges E (the complete graph with loops added at every vertex). At every vertex there are exactly $(n-1) + 2 = n + 1$ incident edges, since a loop counts as 2. Since this number is even there is an Eulerian cycle $v_1, \dots, v_N, v_{N+1} = v_1$ in G [Gondran and Minoux (1984), Theorem 1, page 338], which we may assume has $1 = v_1 = v_N$. If k is even, let $(a(k), b(k)) = (v_k, v_{k+1})$ and if k is odd, let $(a(k), b(k)) = (v_{k+1}, v_k)$. In vertical notation, the ordering of E looks like:

$$\begin{array}{lccccccccc} b(k) \to & 1 & v_3 & v_3 & \cdots & v_k & v_{k+2} & v_{k+2} & \cdots & 1 \\ a(k) \to & v_2 & v_2 & v_4 & \cdots & v_{k+1} & v_{k+1} & v_{k+3} & \cdots & 1 \end{array}.$$

Observe that all occurrences of every label i appear in pairs, with the possible exception of the four 1's in columns 1, $N-1$ and N. If $n = 1$ (mod 4), then N is odd and the 1 in column $N-1$ is in the top row, so the pairing holds for all the 1's, too. Since each label i occurs $n+1$ times, it occurs in $(n+1)/2$ contiguous pairs and we are done. If $n = 3$ (mod 4), then there is a 1 in the bottom row of column $N-1$, so these four 1's are still in two contiguous sets and the occurrences of any label i still form at most $(n+1)/2$ contiguous sets, as required.

If n is even, the graph G has odd degree $(n+1)$ at every vertex. In this case, define G' to be the multigraph with $N' = N + n/2$ edges obtained from G by adding another copy of each edge $(1,2), (3,4), \dots, (n-1, n)$. Observe that every vertex has even degree $n+2$ in G'. Apply the same argument as before to obtain N' columns with all labels (except possibly 1, which is treated specially, as before) appearing $n+2$ times in $(n+2)/2$ pairs. Then delete one appearance each, for the $n/2$ added columns (edges). Renumber the columns and in the resulting circular ordering each label appears in at most $(n+2)/2$ contiguous sets. □

EXAMPLE 1 ($n = 3$, $N = 6$). An Eulerian cycle in G is given by 1, 2, 2, 3, 3, 1. The associated ordering of E, writing pairs vertically, is given by

$$\begin{matrix} 1 & 2 & 2 & 3 & 3 & 1 \\ 2 & 2 & 3 & 3 & 1 & 1 \end{matrix} \quad \text{(two contiguous sets)}.$$

EXAMPLE 2 ($n = 4$, $N = 10$, $N' = 12$). An Eulerian cycle in G' is given by 1, 2, 2, 3, 3, 4, 4, 1, 3, 4, 2, 1. If we delete the second occurrence of the additional edges (1, 2) and (3, 4) (marked x), the ordering works.

$$\begin{matrix} 1 & 2 & 2 & 3 & 3 & 4 & 4 & 3 & 3 & 2 & 2 & 1 \\ 2 & 2 & 3 & 3 & 4 & 4 & 1 & 1 & 4 & 4 & 1 & 1 \\ & & & & & & & & x & & x & \end{matrix} \quad \text{(three contiguous sets)}.$$

THEOREM 1. *If R is a symmetric matrix, then P has a rotational representation $(\frac{1}{2}, S)$ where S has type $[n/2] + 1$.*

PROOF. As R is a symmetric matrix, it is a convex combination of n cycle matrices of length one and $n(n-1)/2$ cycle matrices of length two with coefficients r_{ii} in the (i) cycle and $2r_{ij}$ in the (i, j) cycle. Let $(a(i), b(i))$, $i = 1, \ldots, N$ be as in Lemma 1.

Define

$$\alpha_0 = 0,$$
$$\alpha_i = (r_{a(i), b(i)})/2 \quad \text{if } a(i) = b(i),$$
$$\alpha_i = r_{a(i), b(i)} \quad \text{if } a(i) \neq b(i), i = 1, 2, \ldots, N.$$

Let A_{k1}, $k = 1, \ldots, N$ be a partition of $[0, \frac{1}{2})$, where

$$A_{k1} = \left[\sum_{i=0}^{k-1} \alpha_i, \sum_{i=0}^{k} \alpha_i \right).$$

Define $A_{k2} = f_{1/2}(A_{k1})$, $k = 1, \ldots, N$,

$$S_i = \left(\bigcup_{a(k)=i} A_{k1} \right) \cup \left(\bigcup_{b(k)=i} A_{k2} \right), \qquad S = \{S_i\}_{i=1, \ldots, n}.$$

Note that

$$R = \sum_{k=1}^{N} 2\alpha_k C_{(a(k), b(k))},$$

where $C_{(a(k), b(k))}$ is the $n \times n$ cycle matrix with elements:

$$\text{if } a(k) \neq b(k),\ c_{a(k), b(k)} = c_{b(k), a(k)} = \tfrac{1}{2}; \qquad c_{ij} = 0 \text{ otherwise},$$
$$\text{if } a(k) = b(k),\ c_{a(k), b(k)} = 1; \qquad c_{ij} = 0 \text{ otherwise}.$$

Direct calculus proves that $(\frac{1}{2}, S)$ is a rotational representation of P. The assignment of labels $(a(k), b(k))$ shows that S has type $[n/2] + 1$. □

In case the matrix R does not contain all possible cycles of length two or all possible cycles of length one, fewer subintervals in the previous construction are required and the type of the partition may possibly be less than $[n/2] + 1$. For example, if $p_{ii} = 0$, $i = 1, \dots, n$ (i.e., there are not any loops) and n is even or $n = 3 \pmod 4$, then the matrix P has a rotational representation in which the partition S has type $[n/2]$.

3. Relations between the rotational representation of a recurrent stochastic matrix and its reversed matrix. Let P be a $n \times n$ recurrent matrix with v its stationary vector. Let $Q = (q_{ij})$ be defined $q_{ij} = (v_j p_{ji})/v_i$. Q is called the reversed matrix of P. It is well known that Q is a stochastic matrix with a stationary vector v.

LEMMA 2. *Let (t, S) be a rotational representation of P. Then $(1 - t, S)$ is a rotational representation of Q.*

PROOF. Let $f_t(x) = (x + t)(\mathrm{mod}\, 1)$, $g_t(x) = (x + 1 - t)(\mathrm{mod}\, 1)$ be shift transformations on $[0, 1)$. It is very easy to show that $f_t = g_t^{-1}$. As (t, S) is a rotational representation of P, then $p_{ij} = (m(f_t(S_i) \cap S_j))/m(S_i)$. And $q_{ij} = (v_j p_{ji})/v_i = m(f_t(S_j) \cap S_i)/m(S_i) = m(S_j \cap g_t(S_i))/m(S_i)$. So the lemma is proved. □

THEOREM 2. *A recurrent matrix P is reversible if and only if it has a rotational representation $(\frac{1}{2}, S)$, for some partition S. If so, there is such a representation where the type of S is $[n/2] + 1$.*

PROOF. Let P be a recurrent reversible matrix, then $p_{ij} = q_{ij}$, so R is symmetric and we apply Theorem 1. Conversely, suppose that P has a rotational representation $(\frac{1}{2}, S)$, then by Lemma 2, Q has the same representation, so $P = Q$. □

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