A GEOMETRIC REPRESENTATION OF A STOCHASTIC MATRIX: THEOREM AND CONJECTURE

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An irreducible stochastic matrix may be constructed by partitioning a line of unit length into a finite number of intervals, shifting the line to the right (mod 1) by a small amount, and defining transition probabilities in terms of the overlaps among the intervals before and after the shift. It is proved that every $2 \times 2$ irreducible stochastic matrix arises from this construction. Does every $n \times n$ irreducible stochastic matrix arise this way?

A stochastic matrix $P$ is an $n \times n$ matrix with nonnegative real elements $p_{ij}$ such that every row sum is 1. We assume $1 < n < \infty$. We shall describe a simple geometric construction, based on partitioning and mapping the unit interval, that produces an irreducible stochastic matrix. A matrix $P$ is irreducible if and only if, for any row $i$ and any column $j \neq i$, there exists a positive integer $k$, which may depend on $i$ and $j$, such that the $i,j$ element of $P^k$ is not zero. Whenever such a $k$ exists, it may be chosen to be less than $n$. We shall show that every irreducible $2 \times 2$ stochastic matrix arises from such a construction.

We have neither a proof nor a counterexample to the conjecture that every irreducible $n \times n$ stochastic matrix, $n > 2$, also arises from this construction. We offer the conjecture as an open problem.

A theorem of Alpern (1978) gives a geometric representation of every primitive stochastic matrix. A stochastic matrix $P$ is primitive if, for some positive integer $k$, every element of $P^k$ is positive. Our conjectured geometric representation would simplify certain special cases of his theorem, which we describe in more detail later.

In addition, our conjecture, if true, would reveal an attractively simple structure in irreducible stochastic matrices.

We now describe a geometric construction that produces an irreducible stochastic matrix.

Let $X$ be the unit interval $[0, 1)$. Partition $X$ into $n$ sets $J_1, \ldots, J_n$ each of positive Lebesgue measure. Suppose each $J_i$ is the union of $n-1$ intervals $I_a = [x_a^L, x_a^R)$, where $[a, b) = \emptyset$ if $b \leq a$. The superscripts $L$ and $R$ identify the left and right endpoints. We will explain later why we choose $n-1$ intervals, rather than some other number, to compose each $J_i$. In case $n = 2$, $J_1 = I_{i_1}$, $i = 1, 2$ and we may take $J_1 = [0, x_1), J_2 = [x_1, 1)$ for some $x_1$ in $(0, 1)$. For any $t$ and $x$ in $X$, let

$$f_t(x) = (x + t)(\mod 1),$$

that is, $f_t(x)$ is the fractional part of $x + t$. $f_t$ preserves Lebesgue measure, which we denote by $m$: $m(I_{i_k}) = x_{i_k}^R - x_{i_k}^L$.

Define

$$p_{ij} = m(f_t(I_{i_j}) \cap J_j)/m(J_i).$$

Since $f_t$ is measure-preserving, (1) is the same as

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Received June 9, 1980; revised September 16, 1980.

1 This work was partially supported by N.S.F. grant DEB 80-11026.


Key words and phrases. Measure-preserving transformation, ergodic theory, mapping of the unit interval, Markov chain.
\[ p_{ij} = \frac{m(f_i(J_i) \cap J_j)}{m(f_i(J_i))}. \]

Since \( m \geq 0 \) and \( m(J_i) > 0 \) by assumption, \( p_{ij} \) is well defined and non-negative. Also \( \sum_{j=1}^{n} p_{ij} = \frac{m(f_i(J_i) \cap \bigcup J_j)}{m(J_i)} = \frac{m(f_i(J_i))}{m(J_i)} = 1. \) So \( P = (p_{ij}) \) is stochastic. In case \( n = 2 \) and \( 0 < t < 1, \) \( P \) is irreducible.

Let \( \pi \) be a row \( n \)-vector with \( \pi_i = m(J_i), \ i = 1, \ldots, n. \) Then the \( j \)th element of \( \pi P \) is \( \sum_i \pi_i p_{ij} = \sum_i m(f_i(J_i) \cap J_j) = m(J_j) = \pi_j. \) Hence \( \pi P = \pi. \) Thus we can construct a stochastic matrix \( P \) with an arbitrary invariant distribution \( \pi > 0 \) by choosing \( J_i \) such that \( \pi_i = m(J_i). \)

An \( n \times n \) positive stochastic matrix can be represented by a representation of the form \( \sum_{j=1}^{n} (\pi_j J_j) = \bigcup J_j. \) A reducible stochastic matrix \( M \) has either no representation or an infinity of representations because \( f_0(J_2) = J_2 \) has no intersection with \( J_1. \)

Let \( \pi = \pi(J_1) \) be an irreducible \( 2 \times 2 \) stochastic matrix. \( M \) is irreducible if and only if both elements off the main diagonal are not zero. There exists a positive row vector \( v \) such that \( vM = v \) (Seneta, 1973). Assume \( v_1 + v_2 = 1. \) It may be checked that

\[ v = (m_{12}/(m_{12} + m_{21}), m_{22}/(m_{12} + m_{21})). \]

We will show how to find \( J_1, J_2 \) and \( t > 0 \) such that \( m_{ij} = p_{ij} \) where \( p_{ij} \) is given by (1). Since \( v \) is the invariant distribution of \( M \) and of the desired \( P, \) it is natural, in the light of the above, to let \( J_1 = [0, v_1), J_2 = [v_1, 1). \)

Let

\[ t = m_{12} m_{22}/(m_{12} + m_{21}). \]

Since \( M \) is irreducible, \( t > 0. \) Comparing (2) and (3) shows that \( t \leq v_i, \ i = 1, 2, \) because \( m_{ij} \leq 1, i \neq j. \)

Now \( f_i(J_i) \cap J_1 = [t, v_1 + t) \cap [0, v_1) = [v_1, v_1 + t) \cap [0, v_1) \) so \( m(f_i(J_i) \cap J_1) = v_1 - t \) and by (1),

\[ p_{11} = (v_1 - t)/v_1. \]

Substituting (2) and (3) into the right side of (4) yields \( p_{11} = m_{11} \) as desired. It follows that \( p_{12} = m_{12}. \) Since \( t > 0, \) \( p_{11} < 1 \) and \( p_{12} > 0. \)

Similarly, \( f_i(J_2) \cap J_2 = ([v_1 + t, 1) \cup [0, t)) \cap [v_1, 1) = [v_1 + t, 1) \cup [v_1, t). \) But \( [v_1, t) = \emptyset \) because \( t \leq v_1. \) Thus \( m(f_i(J_2) \cap J_2) = 1 - v_1 - t = v_2 - t < v_2. \) By (1), using (2) and (3) as before,

\[ p_{22} = (v_2 - t)/v_2 = m_{22}. \]

We have shown that for any irreducible stochastic \( 2 \times 2 \) matrix \( M, \) there exists a representation of the form (1), with \( 0 < t < 1. \) Since \( M \) and the representation (1) each have exactly 2 degrees of freedom (e.g., \( m_{12} \) and \( m_{21} \) in \( M \) and \( t \) and \( v_1 \) in (1)), the representation is unique, except possibly for a cyclic permutation of \( J_1 \) and \( J_2. \)

What happens if a \( 2 \times 2 \) stochastic matrix \( M \) is reducible? Then at least one off-diagonal element, say \( m_{12}, \) is 0. If we seek a representation in the form (1), then \( p_{12} = 0 \) implies \( t = 0, \) however \( J_1 \) and \( J_2 \) are chosen. Now if \( m_{21} \neq 0, \) then no representation (1) is possible because \( f_0(J_2) = J_2 \) has no intersection with \( J_1. \) If \( m_{21} = 0, \) then a representation (1) exists for every partition of \( X \) into intervals \( J_1, J_2 \) of positive length because \( P = M = I. \) Thus a reducible stochastic matrix \( M \) has either no representation or an infinity of representations of the form (1).

To see why we suppose each \( J_i \) is the union of \( n - 1 \) intervals, consider the positive \( n \times n \) matrix \( M \) with \( m_{ij} = 1 - nd, \ m_0 = d, i, j = 1, \ldots, n, i \neq j, \) for \( 0 < nd < 1 \) and \( n > 2. \) Take \( d \) very small. Since the diagonal elements of \( M \) then approach 1, \( (\text{mod } 1) \) must also become very small. Now suppose \( J_i, \) say, consisted of \( n - 2 \) or fewer intervals \( I_{ik}. \) Then the \( n - 2 \) or fewer intervals that lie just to the right (\text{mod } 1) of each \( I_{ik} \) could belong to at most \( n - 2 \) different \( J_i, i \neq 1. \) Hence for small enough \( t, \) there would have to be at least one \( p_{1k} = 0, k \neq 1, \) according to (1). Thus if \( J \) consists of fewer than \( n - 1 \) intervals, not every positive stochastic matrix can be represented by (1). We conjecture that \( J \) need contain no more than \( n - 1 \) intervals because we know no argument why more should be required.
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For every irreducible stochastic matrix of order $3 \times 3$ or larger, does a representation in the form (1) exist? If a representation exists, under what conditions, if any, is it unique (up to cyclic permutations of the set of all $I_a$ in $X$)?

A special case of a result due to Alpern (1978, page 18) may be stated as follows. Let $P$ be a primitive stochastic matrix. Let $g$ be an invertible aperiodic $m$-preserving transformation of $X$. (For example, every $f_i$ with $t$ irrational is such a $g$.) Then there exists a partition $H_1, \ldots, H_n$ of $X$ such that $m(g(H_i) \cap H_i)/m(H_i) = p_{ij}$. This result is stronger than our conjecture in guaranteeing that for every $g$, a partition $(H_i)$ exists that represents a given $P$. This result is weaker than our conjecture in assuming $P$ primitive and in permitting $H_i$ to be any measurable subset of $X$, rather than only a union of $n - 1$ intervals like $J_i$.

The definition of $f_i(x)$ suggests a stochastic process that mimics the marginal frequencies and one-step transition probabilities of a stationary Markov chain specified by (1). Let $U_0$ be uniformly distributed on [0, 1) and let, for every positive integer $k$, $U_k = (U_{k-1} + t) \pmod 1$. Let $Z_k = i$ if $U_k \in J_i$, $k = 0, 1, 2, \ldots$. Then $P[Z_0 = i] = \pi_i$ and $P[Z_{k+1} = j | Z_k = i] = p_{ij}$, $k = 0, 1, \ldots$. A referee asks: is $(Z_k)$ Markovian? To see that the answer is no, in general, let

$$M = \begin{pmatrix} \frac{1}{6} & \frac{1}{6} \\ \frac{1}{6} & \frac{1}{6} \end{pmatrix},$$

with $\pi = (\frac{1}{6}, \frac{1}{6})$ and $t = \frac{1}{3}$. Then $P[Z_0 = 1, Z_1 = 2] = \frac{1}{12}$ and $P[Z_0 = 1, Z_1 = 2, Z_2 = 1] = 0$ so $P[Z_2 = 1 | Z_1 = 2, Z_0 = 1] = 0$. However, $P[Z_0 = 2, Z_1 = 2] = \frac{1}{12}$ and $P[Z_0 = 2, Z_1 = 2, Z_2 = 1] = \frac{1}{12}$ so $P[Z_2 = 1 | Z_1 = 2, Z_0 = 2] = \frac{1}{6}$.

REFERENCES