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New Methods for Determining Quasi-Stationary Distributions for Markov Chains

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Abstract—We shall be concerned with the problem of determining quasi-stationary distributions for Markovian models directly from their transition rates Q. We shall present simple conditions for a μ-invariant measure m for Q to be μ-invariant for the transition function, so that if m is finite, it can be normalized to produce a quasi-stationary distribution.

Keywords—Markov chains, Stochastic models, Quasi-stationary distributions.

1. INTRODUCTION

In a recent paper, Hart and Pollett [1] identified conditions, expressed solely in terms of the transition rates Q of a continuous-time Markov chain, which guarantee that *any* finite μ-invariant measure for Q can be normalized to produce a quasi-stationary distribution. These *Reuter FE conditions* (so named because of their similarity to Reuter's [2] conditions for the forward differential equations to have a unique solution) extended and complemented earlier work [3–8] on the relationship between μ-invariant measures and quasi-stationary distributions. The Reuter FE conditions involve testing for the nonexistence of a solution to an infinite system of linear equations, but, for a range of specific models, they can usually be expressed in quite simple terms. For example, in the case of birth-death processes, they are expressed in terms of the divergence of certain series [1]. Since the transition rates of a birth-death process are *reversible* with respect to a measure π, one might hope for a simplification of the Reuter FE conditions in the more general case of reversible Markov chains. This is indeed the case, and our main result, presented in Section 3, establishes that if Q is reversible with respect to a subinvariant measure π, then every μ-invariant measure for Q which is bounded above by π is also μ-invariant for the transition function. We shall illustrate this result with reference to some simple Markovian models, including the birth-death process. Further examples have appeared in [9]. Finally, in Section 4, we shall indicate how the reversibility assumption can be relaxed, thus providing a set of analogous conditions for general Markov chains.

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We begin by reviewing the existing theory of μ-invariant measures and quasi-stationary distributions for continuous-time Markov chains.

2. QUASI-STATIONARY DISTRIBUTIONS

Let $S = \{0, 1, \dots\}$ and let $Q = (q_{ij},\ i, j \in S)$ be a stable, conservative, and regular q-matrix of transition rates over S. Let $(X(t),\ t \geq 0)$ be the unique Markov chain associated with Q and denote its transition function by $P(\cdot) = (p_{ij}(\cdot),\ i, j \in S)$. Let C be a subset of S and μ some fixed nonnegative real number. Then, the measure $m = (m_j, j \in C)$ is called a *μ-invariant measure for P* if

$$\sum_{i\in C} m_i p_{ij}(t) = e^{-\mu t} m_j, \qquad j \in C, \quad t \geq 0. \tag{2.1}$$

In contrast, m is called a *μ-invariant measure for Q* if

$$\sum_{i\in C} m_i q_{ij} = -\mu m_j, \qquad j \in C. \tag{2.2}$$

We shall take $C = \{1, 2, \dots\}$ and for simplicity we shall suppose that C is irreducible; this guarantees that all nontrivial μ-invariant measures m satisfy $m_j > 0$ for all $j \in C$. We shall also assume that 0 is an absorbing state, that is $q_{00} = 0$, and that $q_{i0} > 0$ for some $i \in C$, a condition which guarantees a positive probability of absorption starting in i. We shall use van Doorn's [10] definition of a quasi-stationary distribution.

DEFINITION. *Let $m = (m_j,\ j \in C)$ be a probability distribution over C and define $h(\cdot) = (h_j(\cdot),\ j \in S)$ by*

$$h_j(t) = \sum_{i\in C} m_i p_{ij}(t), \qquad j \in S, \quad t \geq 0. \tag{2.3}$$

Then, m is a quasi-stationary distribution if, for all $t > 0$ and $j \in C$,

$$\frac{h_j(t)}{\sum_{i\in C} h_i(t)} = m_j.$$

That is, if the chain has m as its initial distribution, then m is a quasi-stationary distribution if the state probabilities at time t, conditional on the chain being in C at t, are the same for all t.

The relationship between quasi-stationary distributions and the transition probabilities of the chain was identified by Nair and Pollett [4]. They showed that a probability measure $m = (m_j,\ j \in C)$ over C is a quasi-stationary distribution if and only if, for some $\mu > 0$, m is a μ-invariant measure for P. Thus, in a way which mirrors the theory of *stationary distributions*, quasi-stationary distributions can be interpreted as eigenvectors of the transition function. However, the transition function is available explicitly in only a few simple cases, and so one requires a means of determining quasi-stationary distributions directly from transition rates of the chain. Since q_{ij} is the right-hand derivative of $p_{ij}(\cdot)$ near 0, an obvious first step is to rewrite (2.1) as

$$\sum_{i\in C: i\neq j} m_i p_{ij}(t) = \left((1 - p_{jj}(t)) - \left(1 - e^{-\mu t}\right)\right) m_j, \qquad j \in C, \quad t \geq 0.$$

Then, proceeding formally, dividing this expression by t and letting $t \downarrow 0$, we arrive at (2.2). This argument can be justified rigorously (see [11, Proposition 2]), and so if m is a quasi-stationary distribution then, for some $\mu > 0$, m is a μ-invariant measure for Q.

The more interesting question of when a positive solution m to (2.2) is also a solution to (2.1) was answered in [12,13].

THEOREM 1. *A μ-invariant measure m for Q is μ-invariant for P if and only if the equations*

$$\sum_{i\in C} y_i q_{ij} = \nu y_j, \qquad 0 \leq y_j \leq m_j, \quad j \in C, \tag{2.4}$$

have no nontrivial solution for some (and then for all) $\nu > -\mu$.

Thus, the problem of determining μ-invariant measures, and hence, quasi-stationary distributions, was ostensibly solved, but conditions (2.4) were found to be difficult to verify in practice. Consequently, a range of simpler sufficient conditions were sought. The first of these was based on the premise that the μ-invariant measure m for Q be finite; [8] showed that a μ-invariant probability measure for Q is a quasi-stationary distribution if and only if $\mu = \sum_{i\in C} m_i q_{i0}$, a condition which stipulates that μ be equal to the *probability flux* into the absorbing state under m. However, although these conditions have proved useful in practice [14,15], they are deficient in so far as μ and m are interrelated; indeed, there is usually a one-parameter family of quasi-stationary distributions indexed by μ. This problem was addressed by Hart and Pollett [1], who presented a set of conditions solely in terms of the transition rates.

THEOREM 2. THE REUTER FE CONDITIONS. *If the equations*

$$\sum_{i\in C} y_i q_{ij} = \nu y_j, \qquad j \in C,$$

have no nontrivial, nonnegative solution such that $\sum_{i\in C} y_i < \infty$, *for some (and then all)* $\nu > 0$, *then all* μ*-invariant probability measures for* Q *are quasi-stationary distributions.*

The conditions we shall present here for a μ-invariant measure for Q to be μ-invariant for P do not require m to be finite, but rather involve comparing m with a subinvariant measure on C for Q, that is, a measure $\pi = (\pi_j,\ j \in C)$ which satisfies

$$\sum_{i\in C} \pi_i q_{ij} \le 0, \qquad j \in C. \tag{2.5}$$

Our irreducibility assumption guarantees that all nontrivial subinvariant measures satisfy $\pi_j > 0$ for all $j \in C$.

We shall first deal with the case when Q is reversible with respect to π.

3. THE REVERSIBLE CASE

Suppose that there exists a collection of positive numbers $\pi = (\pi_i,\ i \in C)$ satisfying the *detailed-balance conditions*

$$\pi_i q_{ij} = \pi_j q_{ji}, \qquad i,j \in C. \tag{3.1}$$

Then, summing (3.1) over i in C shows that π satisfies (2.5). Thus, π is a subinvariant measure for Q; Q is said to be *reversible with respect to* π.

THEOREM 3. *Suppose that* Q *is reversible with respect to the subinvariant measure* $\pi = (\pi_i,$ $i \in C)$. *Then, every* μ*-invariant measure* $m = (m_i,\ i \in C)$ *for* Q *which is bounded by* π, *that is,*

$$\sup_{i\in C}\left\{\frac{m_i}{\pi_i}\right\} < \infty, \tag{3.2}$$

is also μ*-invariant for* P.

It should be emphasized that neither π nor m need be finite; we require only that m be bounded above by π. If m *is* finite, it can then be normalized to produce a quasi-stationary distribution. Our proof rests heavily on the assumption that Q be regular, a condition which cannot be relaxed under reversibiliy.

PROOF. Let m be a μ-invariant measure which satisfies (3.2) and suppose that m is *not* μ-invariant for P. Then, by Theorem 1, equations (2.4) have a nontrivial solution y, certainly for $\nu > 0$. On substituting (3.1) into (2.4), we find that $z = (z_j,\ j \in C)$, given by $z_j = y_j/\pi_j$, satisfies

$$\sum_{i\in C} q_{ji} z_i = \nu z_j, \tag{3.3}$$

with $0 < z_j \le m_j/\pi_j$ for all $j \in C$. But, m is bounded above by π and so we have found a bounded, nontrivial, nonnegative solution to (3.3). Thus, by Theorem 2.2.7 of [16], we have contradicted our assumption that Q is regular. ∎

EXAMPLE 1. We shall illustrate Theorem 3 with reference to the absorbing birth-death process on $S = \{0, 1, \dots\}$. This has transition rates given by

$$q_{ij} = \begin{cases} \lambda_i, & \text{if } j = i+1, \\ -(\lambda_i + \mu_i), & \text{if } j = i, \\ \mu_i, & \text{if } j = i-1, \\ 0, & \text{otherwise,} \end{cases}$$

where the birth rates $(\lambda_i,\ i \ge 0)$ and the death rates $(\mu_i,\ i \ge 0)$ satisfy $\lambda_i,\ \mu_i > 0$, for $i \ge 1$, and $\lambda_0 = \mu_0 = 0$. Thus, 0 is an absorbing state and $C = \{1, 2, \dots\}$ is an irreducible class. Define series $\mathcal{A}$ and $\mathcal{C}$ by

$$\mathcal{A} = \sum_{i=1}^{\infty} \frac{1}{\lambda_i \pi_i} \qquad \text{and} \qquad \mathcal{C} = \sum_{i=1}^{\infty} \frac{1}{\lambda_i \pi_i} \sum_{j=1}^{i} \pi_j,$$

where $\pi = (\pi_i,\ i \in C)$, given by $\pi_1 = 1$ and $\pi_i = \sum_{j=2}^{i} \lambda_{j-1}/\mu_j$, for $i \ge 2$, is a subinvariant measure on C with respect to which Q is reversible. We shall assume that $\mathcal{C} = \infty$, a condition which is necessary and sufficient for Q to be regular (see [16]). The classical Karlin and McGregor Theory of the birth-death process involves the recursive construction of a sequence of orthogonal polynomials using the equations for an x-invariant vector (see [10]): define $(\phi_i(\cdot),\ i \in C)$, where $\phi_i : \mathrm{R} \to \mathrm{R}$, by $\phi_1(x) = 1$, $\lambda_1 \phi_2(x) = \lambda_1 + \mu_1 - x$, and

$$\lambda_i \phi_{i+1}(x) - (\lambda_i + \mu_i)\phi_i(x) + \mu_i \phi_{i-1}(x) = -x\phi_i(x), \qquad i \ge 2,$$

and let

$$m_i = \pi_i \phi_i(x), \qquad i \in C, \quad x \in \mathrm{R}. \tag{3.4}$$

It can be shown [10] that $\phi_i(x) > 0$ for x in the range $0 \le x \le \lambda$, where λ (≥ 0) is the decay parameter of C (see [17]). Since Q is reversible with respect to π, it follows, from [13, Theorem 4.1 b(ii)], that, for each fixed x in the above range, $m = (m_i,\ i \in C)$ is an x-invariant measure for Q; specifically, m satisfies (2.2) with $\mu = x$. Moreover, m is uniquely determined up to constant multiples. We can use Theorem 3 to obtain conditions under which m is μ-invariant for P. In view of (3.4) we need simply to determine whether $\phi_i(x)$ is bounded in i. This is not straightforward, and we thank van Doorn for providing the argument: using Theorems 3.1, 3.4(i), 3.6, and 3.8 of [18], one can show that, for every x in the range $0 \le x \le \lambda$, $\phi_i(x)$ is bounded in i if and only if $\mathcal{A} < \infty$. Thus, the given m is μ-invariant for P if $\mathcal{A} < \infty$. This complements the "classical case" $\mathcal{A} = \infty$ dealt with by van Doorn. Theorem 3.2(i) of [10] establishes that under this condition also, m is μ-invariant for P. Hence, (3.2) is not a necessary condition for m to be μ-invariant for P. These results are now well known; for a detailed analysis see [19].

EXAMPLE 2. Our second example is taken from Jacka and Roberts [20], who used it to show that conditioned Markov chains do not always converge weakly. The q-matrix of the chain is given by

$$q_{10} = \frac{1}{2}, \quad q_{11} = -q_1 = -1, \quad q_{i1} = -q_{ii} = q_i, \qquad \text{for all } i \ge 2,$$
$$q_{1j} > 0, \quad \text{for all } j \ge 2, \quad q_{ij} = 0 \quad \text{otherwise,}$$

where the constants q_i are all positive. Clearly, 0 is an absorbing state accessible via State 1 from the irreducible class $C = \{1, 2, \dots\}$; on leaving State 1 the chain is either absorbed with probability 1/2, or jumps to a higher state j with probability q_{1j} (note that $\sum_{k \ge 2} q_{1k} = 1/2$) and then returns to State 1 after an exponential holding time with mean $1/q_j$, and so forth. It is elementary to show that Q is regular and that $\pi = (\pi_j,\ j \in C)$, given by $\pi_j = q_{1j}/q_j$, is a subinvariant measure on C with respect to which Q is reversible.

Next, a simple calculation based on (2.2) reveals that nontrivial μ-invariant measures m exist for Q if and only if μ satisfies

$$\sum_{k\geq 2} q_{1k}\frac{q_k}{q_k-\mu} = 1-\mu, \tag{3.5}$$

in which case m is given, unique up to constant multiples, by

$$m_i = \frac{q_{1i}}{q_i-\mu}, \qquad i \in C. \tag{3.6}$$

Note, that of necessity $\mu \leq q := \inf_{j\in C} q_j$ (≤ 1) [17], and that clearly

$$\frac{m_i}{\pi_i} = \frac{q_i}{q_i-\mu} \leq \frac{q}{q-\mu}.$$

Now, the right-hand and left-hand sides of (3.5) are monotonically increasing and decreasing, respectively, from $1/2$ and 1, respectively, at $\mu = 0$. So, there is at most one μ which satisfies (3.5). Thus, we have proved that a μ-invariant m exists for Q if and only if

$$\sum_{k\geq 2} q_{1k}\frac{q_k}{q_k-q} \geq 1-q.$$

When this condition holds, m is given by (3.6), with μ being the unique solution to (3.5), and m is μ-invariant for P.

4. A MORE GENERAL RESULT

Theorem 3 can be generalized in a number of ways, but we shall content ourselves with the following result, which requires neither the reversibility of Q with respect to π, nor the regularity of Q. When Q is *not* regular, there is no longer a unique process with transition rates Q, but in such cases we can take P to be the transition function of the *minimal process* [16]. We may also relax the condition that π be a subinvariant measure for Q.

THEOREM 4. *Let $\pi = (\pi_i,\ i \in C)$ be a collection of positive numbers such that the equations*

$$\sum_{i\in C} x_i q_{ij} = \nu x_j, \qquad 0 \leq x_j \leq \pi_j, \quad j \in C, \tag{4.1}$$

have no nontrivial solution for some (and then all) $\nu > 0$. Then, every μ-invariant measure $m = (m_i,\ i \in C)$ for Q which is bounded above by π is also μ-invariant for P.

PROOF. Let m be a μ-invariant measure which satisfies (3.2), but is *not* μ-invariant for P. Then, as before, (2.4) has a nontrivial solution y for $\nu > 0$. Now, y is bounded above by π because m is. Therefore, by setting

$$x_i = \frac{y_i}{\sup_{j\in C}\{y_j/\pi_j\}},$$

we obtain a nontrivial solution $x = (x_i, i \in C)$ to (4.1), thus contradicting the conditions of the theorem. ∎

A convenient choice of π is any subinvariant measure on C for Q. Using this, we can explain why Theorem 3 is a corollary of Theorem 4, and in particular, how the regularity condition of Theorem 3 can be realized as a consequence of Theorem 4. To achieve this, we must define a *reverse* q-matrix $Q^* = (q^*_{ij},\ i,j \in C)$ by setting

$$q^*_{ij} = \frac{\pi_j q_{ji}}{\pi_i}, \qquad i,j \in C. \tag{4.2}$$

Clearly Q^* is a stable q-matrix over C. If Q^* were conservative over C, that is, if π were *invariant* on C for Q, then the invariance condition (4.1) would be necessary and sufficient for Q^* to be regular. This can be seen on substituting (4.2) into (2.4). If y is a nontrivial solution to (2.4), then $z = (z_i,\ i \in C)$, given by $z_i = y_i/\pi_i$, provides a nontrivial solution to

$$\sum_{j\in C} q^*_{ij} z_j = \nu z_i, \qquad 0 \le z_i \le \frac{m_i}{\pi_i}, \quad i \in C.$$

But, m is bounded above by π, implying that z must be bounded, and hence, that Q^* is not regular. Conversely, if Q^* is not regular, then, for any choice of $\nu > 0$, there exists a nontrivial $z = (z_j,\ j \in C)$ satisfying

$$\sum_{j\in C} q^*_{ij} z_j = \nu z_i, \qquad 0 \le z_i \le 1, \quad i \in C. \tag{4.3}$$

Once again, substituting (4.2) into (4.3) yields $y = (y_i,\ i \in C)$, where $y_i = \pi_i z_i$ as a solution to (4.1). Thus, we have shown that if π is an invariant measure on C for Q and equations (4.1) have no nontrivial solution for some (and then all) $\nu > 0$, then every μ-invariant measure on C for Q which is bounded above by π is also μ-invariant for P. This extends Theorem 1(ii) of [21], who showed that condition (4.1) is sufficient for an *invariant* measure for Q to be invariant for P (the $\mu = 0$ case).

However, Q^* is usually nonconservative, since π will usually be strictly subinvariant for Q, and so it is not yet entirely satisfactory to say that Q^* is playing the role which Q played in Theorem 3. However, if we were to extend the definition of Q^* to S by setting $q^*_{0j} = 0$ for $j \in S$ and $q^*_{i0} = -\sum_{j\in C} \pi_j q_{ji}/\pi_i$ for $i \in C$, then Q^* would be conservative over S. Now, by Theorem 2.2.7 of [16], Q^* is regular if and only if the equations

$$\sum_{j\in S} q^*_{ij} z_j = \nu z_i, \qquad 0 \le z_i \le 1, \quad i \in S, \tag{4.4}$$

have only the trivial solution for some (and then all) $\nu > 0$. But, for $i = 0$, $\nu > 0$ implies that $z_0 = 0$ and so (4.4) reduces to (4.3). Thus, as before, (4.1) and (4.3) are equivalent, and so Q^* plays the role which Q played in Theorem 3. Moreover, in the reversible case, $Q^* = Q$ (even for Q^* extended to S), condition (4.1) is necessary and sufficient for Q to be regular. Thus, we see that Theorem 3 is a corollary of Theorem 4.

EXAMPLE 3. Let Q be the q-matrix of a linear birth-death and catastrophe process on $S = \{0, 1, \dots\}$

$$q_{ij} = \begin{cases} 0, & \text{if } j-1 > i > 0 \text{ or } i = 0, \\ \rho i f_{i-j}, & \text{if } 1 \le j \le i-1 \text{ or } i+1 = j > 0, \\ -\rho i(1 - f_0), & \text{if } j = i > 0, \\ \rho i \sum\limits_{k\ge i} f_k, & \text{if } i > j = 0, \end{cases}$$

where $(f_k,\ k = -1, 0, 1, \dots)$ is the left-shifted offspring distribution for the process and $\rho > 0$ is the rate parameter. Assume that $f_0 = 0$, $f_{-1} > 0$, and $f_k > 0$ for some $k > 0$. Under these conditions, 0 is the sole absorbing state and $C = \{1, 2, \dots\}$ is an irreducible, transient class.

We shall make the following definitions:

$$\begin{aligned} f(s) &:= \sum_{k=0}^{\infty} f_{k-1} s^k, \\ b(s) &:= f(s) - s, \\ e &:= f'(1-) = \sum_{k=1}^{\infty} k f_{k-1}, \end{aligned}$$

$$D := 1 - e = 1 - f'(1-) = -b'(1-),$$
$$q := \inf\{s \in (0,1] : f(s) = s\}, \qquad \text{and}$$
$$d := 1 - f'(q-) = -b'(q-).$$

The process is classified as subcritical, critical, or supercritical according as the drift parameter D is negative, zero, or positive.

Let $\pi_i = 1/i$ for $i \in C$. It is easy to check that $\pi = (\pi_i,\ i \in C)$ is a subinvariant measure on C for Q. Now, $m = (m_i,\ i \in C)$, where $m_i = q^i$ is known to be λ-invariant for Q, where $\lambda = \rho d$ is the decay parameter of C for P (see, for example, [22, Theorem 6.3]). If $D \geq 0$, then $q = 1$ and so $\{m_i/\pi_i\}$ is unbounded. On the other hand, if $D < 0$, then $q < 1$ and

$$\frac{m_i}{\pi_i} = iq^i \leq \sum_{j \in C} jq^j = \frac{q}{1-q} < \infty,$$

for all $i \in C$. Thus, if the birth-death and catastrophe process is subcritical, the measure m is bounded above by π. In addition, m is finite and so, provided that it is λ-invariant for P, it can be normalized to obtain a quasi-stationary distribution for the process.

Let $y = (y_i,\ i \in C)$ satisfy (4.1) and consider Q^*, the reverse of Q with respect to π on C. Extend the definition of Q^* to S according to the discussion immediately following the proof of Theorem 4. Then,

$$q^*_{ij} = \begin{cases} 0, & \text{if } 0 \leq j < i-1 \text{ or } j = 0, \\ -\rho i(1 - f_0), & \text{if } j = i \geq 1, \\ \rho i f_{j-i}, & \text{if } j \geq i-1 \text{ and } j \neq i. \end{cases}$$

Note that Q^* is the q-matrix of a Markov branching process P^* which, by Theorem 2.1 of [23], satisfies $jp_{ij}(t) = ip^*_{ji}(t)$, $i, j \in C$. We have already seen that y satisfies (4.1) if and only if $z = (z_i,\ i \in C)$ satisfies (4.3), where $z_i = y_i/\pi_i = iy_i$, $i \in C$. Thus, the invariance condition of Theorem 4 will be satisfied if and only if Q^* is regular, that is, P^* is honest. Theorem 3.3.3 of [16] gives necessary and sufficient conditions for this to be so, namely, that either $e < \infty$, or $e = \infty$ and, for some (and then all) $\varepsilon \in (q,1)$, $\int_\varepsilon^1 (1/b(u))du = -\infty$. Since m is only bounded by π when P is subcritical, the first of these conditions may be refined to $1 < e < \infty$, since $D < 0$ if and only if $e > 1$.

We have proved, for a subcritical birth-death and catastrophe process, that m, given by $m_i = q^i$ for $i \in C$, is a λ-invariant measure on C for P, where $\lambda = \rho d$, if either

(1) $1 < e < \infty$, or

(2) $e = \infty$ and for some (and then all) $\varepsilon \in (q,1)$, $\int_\varepsilon^1 (1/b(u))\,du = -\infty$.

While this example serves to illustrate Theorem 3 and the role played by Q^*, it should be noted that the given m is *always* λ-invariant for P in the subcritical case. By Corollary 1 of [24], the birth-death and catastrophe process is always regular, and since

$$\sum_{i \in C} m_i q_i = \rho \sum_{i=1}^{\infty} iq^i < \infty,$$

(where $q_i = -q_{ii}$), Fubini's Theorem implies that $\sum_{i \in C} m_i q_{i0} = \lambda \sum_{i \in C} m_i$. Thus, by Corollary 1 of [8], m is λ-invariant for P. For further details, see [5] or the proof of Theorem 5.1 of [23]; for details of the supercritical case, see [25].

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