NEW METHODS FOR DETERMINING QUASISTATIONARY DISTRIBUTIONS FOR MARKOV CHAINS

A.G. Hart and P.K. Pollett

Department of Mathematics
The University of Queensland
Queensland Australia

ABSTRACT

We shall be concerned with the problem of determining quasistationary 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 quasistationary distribution.

MARKOV CHAINS; STOCHASTIC MODELS; QUASI-STATIONARY DISTRIBUTIONS
AMS 1991 SUBJECT CLASSIFICATION: PRIMARY 60J27
SECONDARY 60J35

1 INTRODUCTION

In a recent paper, Hart and Pollett (1996) 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 quasistationary distribution. These *Reuter FE conditions* (so named because of their similarity to Reuter's (1957) conditions for the forward differential equations to have a unique solution) extended and complemented earlier work (Elmes, et al. (1994), Nair and Pollett (1993), Pollett (1993a, 1993c, 1995a), Pollett and Vere-Jones (1992)) on the relationship between μ-invariant measures and quasistationary distributions. The Reuter FE conditions involve testing for the non-existence 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 (Hart and Pollett (1996)). 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 will appear in Hart (1997). 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.

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

2 QUASISTATIONARY DISTRIBUTIONS

Let $S = \{0, 1, \ldots\}$ 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 non-negative real number. Then, the measure $m = (m_j,\ j \in C)$ is called a *μ-invariant measure for P* if

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

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 $C = \{1, 2, \ldots\}$ and for simplicity we shall suppose that C is irreducible; this guarantees that all non-trivial 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 at least one $i \in C$, a condition which guarantees a positive probability of absorption starting in i. We shall use van Doorn's (1991) definition of a quasistationary 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*

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

Then, m is a quasistationary 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 quasistationary 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 quasistationary distributions and the transition probabilities of the chain was identified by Nair and Pollett (1993). They showed that a probability measure $m = (m_j,\ j \in C)$ over C is a quasistationary 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*, quasistationary 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 quasistationary 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

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

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 Proposition 2 of Tweedie (1974)), and so if m is a quasistationary 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 Pollett (1986, 1988):

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

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

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

Thus, the problem of determining μ-invariant measures, and hence quasistationary distributions, was ostensibly solved, but the 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; Pollett and Vere-Jones (1992) showed that a μ-invariant probability measure for Q is a quasistationary 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 (Pollett (1993b, 1995b)), they are deficient in so far as μ and m are interrelated; indeed, there is usually a one-parameter family of quasistationary distributions indexed by μ. This problem was addressed by Hart and Pollett (1996), who presented a set of conditions solely in terms of the transition rates:

Theorem 2. (The Reuter FE conditions) *If the equations*

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

have no non-trivial, non-negative 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 quasistationary 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

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

Our irreducibility assumption guarantees that all non-trivial 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 above by π, that is,*

$$\sup_{i \in C} \{m_i/\pi_i\} < \infty, \tag{3.2}$$

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 quasistationary distribution. Our proof rests heavily on the assumption that Q be regular, a condition which cannot be relaxed under reversibility.

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, the equations (2.4) have a non-trivial 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, non-trivial, non-negative solution to (3.3). Thus, by Theorem 2.2.7 of Anderson (1991), 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 $S = \{0, 1, \ldots\}$. 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 $C = \{1, 2, \ldots\}$ is an irreducible class. Define series A and C by

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

where $\pi = (\pi_i,\ i \in C)$, given by $\pi_1 = 1$ and $\pi_i = \prod_{j=2}^{i} \lambda_{j-1}/\mu_j$ for $i \geq 2$, is a subinvariant measure on C with respect to which Q is reversible. We shall assume that $C = \infty$, a condition which is necessary and sufficient for Q to be regular (see Anderson (1991)). 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 van Doorn (1991)): 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

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

and let

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

It can be shown (van Doorn (1991)) that $\phi_i(x) > 0$ for x in the range $0 \leq x \leq \lambda$, where λ (≥ 0) is the decay parameter of C (see Kingman (1963)). Since Q is reversible with respect to π, it follows, from Theorem 4.1 b(ii) of Pollett (1988), 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 Erik van Doorn for providing the argument: using Theorems 3.1, 3.4(i), 3.6 and 3.8 of Kijima and van Doorn (1995), one can show that, for every x in the range $0 \leq x \leq \lambda$, $\phi_i(x)$ is bounded in i if and only if $A < \infty$. Thus, the given m is μ-invariant for P if $A < \infty$. This complements the "classical case" $A = \infty$ dealt with by van Doorn. Theorem 3.2(i) of van Doorn (1991) 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 Kijima et al. (1997).

Example 2. Our second example is taken from Jacka and Roberts (1995), who used it to show that conditioned Markov chains do not always converge weakly. The q-matrix of the chain is given by

$$q_{10} = 1/2; \quad q_{11} = -q_1 = -1; \quad q_{i1} = -q_{ii} = q_i \text{ for all } i \geq 2;$$

$$q_{1j} > 0 \text{ for all } j \geq 2; \quad q_{ij} = 0 \text{ otherwise,}$$

where the constants q_i are all positive. Clearly 0 is an absorbing state accessible via state 1 from the irreducible class $C = \{1, 2, \ldots\}$; 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 $\sum_{k\geq 2} q_{1k} = 1/2$) 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 non-trivial 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) (Kingman (1963)), 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* (Anderson (1991)).

Theorem 4. *Let $\pi = (\pi_i,\ i \in C)$ be a subinvariant measure on C for Q and suppose that the equations*

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

have no non-trivial 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 non-trivial 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 non-trivial solution $x = (x_i,\ i \in C)$ to (4.1), thus contradicting the conditions of the theorem. □

It will not be immediately clear 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 see this, we must define a *reverse* q-matrix $Q^* = (q^*_{ij},\ i, j \in C)$ by setting

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

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

$$\sum_{j \in C} q^*_{ij} z_j = \nu z_i, \qquad 0 \leq z_i \leq \frac{m_i}{\pi_i},\ i \in C. \tag{4.3}$$

But, m is bounded above by π, implying that z must be bounded and hence that Q^* is not regular. However, Q^* is usually non-conservative, 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 π and Q to S by setting $\pi_0 = 1$ and allowing the absorbing state to communicate with C by setting $q_{0j} = -\sum_{i \in C} \pi_i q_{ij}$ for $j \in S$, then π would be an *invariant* measure for Q (equality holds in (2.5) for all j, indeed, for all $j \in S$) and Q^*, defined by (4.2) now for $i, j \in S$, would then be conservative. In this way we can see that Q^* plays the role which Q played in Theorem 3.

This extension is not entirely artificial, for in generic models (such as was the case with the birth-death process) π is often realized as an invariant measure for an irreducible version of the model. It is also worth noting that through our extension procedure we make a connection with the invariance conditions of Kelly (1983); condition (4.1) is necessary and sufficient for π to be an invariant measure for P, where the obvious extension of the definition of P to S follows from that for Q.

5 ACKNOWLEDGEMENTS

The authors are grateful to Laird Breyer and Erik van Doorn for valuable comments on this work. We also gratefully acknowledge the financial support of the Australian Research Council and the University of Queensland. The work of the first author was carried out during the period he spent as a Ph.D. student in the Department of Mathematics of the University of Queensland.

References

[1] Anderson, W.J. (1991) Continuous-time Markov chains: an applications oriented approach, Springer-Verlag, New York.

[2] Elmes, S., Pollett, P.K. and Walker, D.M. (1994) Further results on the relationship between μ-invariant measures and quasistationary distributions for continuous-time Markov chains, *Research Report*, Department of Mathematics, University of Queensland.

[3] Hart, A.G. (1997) *Quasistationary distributions for continuous-time Markov chains*, Ph.D. Thesis, The University of Queensland.

[4] Hart, A.G. and Pollett, P.K. (1996) Direct analytical methods for determining quasistationary distributions for continuous-time Markov chains, In (Eds C.

Heyde, Yu. Prohorov, R. Pyke and Z. Rachev) *Proceedings of the 1995 Athens Conference on Applied Probability and Time Series Analysis*, Springer Lecture Notes Series in Statistics, Springer-Verlag, New York (to appear).

[5] Jacka, S.D. and Roberts, G.O. (1995) Weak convergence of conditioned processes on a countable state space, *J. Appl. Probab.* **32**, 902–916.

[6] Kijima, M. and van Doorn, E.A. (1995), Weighted sums of orthogonal polynomials with positive zeros, *J. Comput. Appl. Math.* **65** (to appear).

[7] Kijima, M., Nair, M.G., Pollett, P.K. and van Doorn, E. (1997) Limiting conditional distributions for birth-death processes, *Adv. Appl. Probab.* **29** (to appear).

[8] Kelly, F.P. (1983) Invariant measures and the q-matrix, In (Eds J.F.C. Kingman and G.E.H. Reuter) *Probability, Statistics and Analysis*, London Mathematical Society Lecture Notes Series Vol. 79, pp. 143–160, Cambridge University Press.

[9] Kingman, J.F.C. (1963) The exponential decay of Markov transition probabilities, *Proc. London Math. Soc.* **13**, 337–358.

[10] Nair, M.G. and Pollett, P.K. (1993) On the relationship between μ-invariant measures and quasistationary distributions for continuous-time Markov chains, *Adv. Appl. Probab.* **25**, 82–102.

[11] Pollett, P.K. (1986) On the equivalence of μ-invariant measures for the minimal process and its q-matrix, *Stochastic Process. Appl.* **22**, 203–221.

[12] Pollett, P.K. (1988) Reversibility, invariance and μ-invariance, *Adv. Appl. Probab.* **20**, 600–621.

[13] Pollett, P.K. (1993a) Analytical and computational methods for modelling the long-term behaviour of evanescent random processes, In (Eds D.J. Sutton, C.E.M. Pearce and E.A. Cousins) *Decision Sciences: Tools for Today, Proceedings of the 12th National Conference of the Australian Society for Operations Research*, pp. 514–535, Adelaide, Australian Society for Operations Research.

[14] Pollett, P.K. (1993b) Modelling the long-term behaviour of evanescent ecological systems, In (Ed M. McAleer) *Proceedings of the International Congress on Modelling and Simulation*, Vol. 1, pp. 157–162, Perth, Modelling and Simulation Society of Australia.

[15] Pollett, P.K. (1993c) Recent advances in the theory and application of quasistationary distributions, In (Eds S. Osaki, and D.N.P. Murthy) *Proceedings of the Australia-Japan Workshop on Stochastic Models in Engineering, Technology and Management*, pp. 477–486, Singapore, World Scientific.

[16] Pollett, P.K. (1995a) The determination of quasistationary distributions directly from the transition rates of an absorbing Markov chain, *Math. Computer Modelling* **22**, 279–287.

[17] Pollett, P.K. (1995b) Modelling the long-term behaviour of evanescent ecological systems, *Ecological Modelling* **75** (to appear).

[18] Pollett, P.K. and Vere-Jones, D. (1992) A note on evanescent processes, *Austral. J. Stat.* **34**, 531–536.

[19] Reuter, G.E.H (1957) Denumerable Markov processes and the associated contraction semigroups on l, *Acta Math.* **97**, 1–46.

[20] Tweedie, R.L. (1974) Some ergodic properties of the Feller minimal process, *Quart. J. Math. Oxford* **25**, 485–495.

[21] van Doorn, E.A. (1991) Quasi-stationary distributions and convergence to quasi-stationarity of birth-death processes, *Adv. Appl. Probab.* **23**, 683–700.