Direct analytical methods for determining quasistationary distributions for continuous-time Markov chains

A.G. Hart
P.K. Pollett
The University of Queensland

ABSTRACT We shall be concerned with the problem of determining the quasistationary distributions of an absorbing continuous-time Markov chain directly from the transition-rate matrix Q. We shall present conditions which ensure that any finite μ-invariant probability measure for Q is a quasistationary distribution. Our results will be illustrated with reference to birth and death processes.

QUASISTATIONARY DISTRIBUTIONS; INVARIANT MEASURES; MARKOV CHAINS

1 Introduction

The most useful conditions to date, which guarantee that a μ-invariant probability distribution m be a quasistationary distribution, stipulate that μ should be equal to the probability flux into the absorbing state; see for example [2], [7], [12], [13] and [15]. However, although these conditions have proved useful in practice (see for example [10], [11] and [14]), 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. Here, we address this problem by presenting conditions, solely in terms of the transition rates, which guarantee that *any* finite μ-invariant measure (or, more generally, any which is finite with respect to the absorption probabilities) can be normalized to produce a quasistationary distribution.

Postal Address: Department of Mathematics, The University of Queensland, Queensland 4072, AUSTRALIA.

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We begin by reviewing existing work on the relationship between μ-invariant measures and quasistationary distributions.

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 [18] definition of a quasistationary distribution.

Definition 1. 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 is made more precise in the following proposition [7]:

Proposition 1. Let $m = (m_j,\ j \in C)$ be a probability measure over C. Then, m 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*, one can interpret quasistationary distributions 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 [17]), and so, in view of Proposition 1, we have the following simple result:

Proposition 2. 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 [8, 9]:

Proposition 3. 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) $\nu > -\mu$.

If we seek a quasistationary distribution then the μ-invariant measure m for Q can be taken to be finite, in which case simpler conditions obtain. The following result can be deduced from Theorems 3.2, 3.4 and 4.1 of [7]:

Proposition 4. Let m be a probability measure over C and suppose that m is μ-invariant for Q. Then, m is a quasistationary distribution if and only if $\mu = \sum_{i\in C} m_i q_{i0}$.

3 The Reuter FE Conditions

Our main result gives conditions on Q which guarantee that *any* probability distribution over C which is μ-invariant for Q is a quasistationary distribution:

Theorem 1. If the equations

$$\sum_{i\in C} y_i q_{ij} = \nu y_j, \quad j\in C, \tag{3.5}$$

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 μ-invariant for P.

Remarks. (1) Many of the assumptions we have made can be relaxed. First, Q need not be regular or even conservative; the conclusions of the theorem are valid taking P to be the minimal transition function. Next, C need not be irreducible. For example, we can take C to be the whole of the state space S, which itself need not be of any particular form. More generally, C can be the union of irreducible classes (that is, irreducible with respect to the minimal chain), provided we impose some extra conditions, as follows. If C_1 and C_2 are two such classes with $C_1 \prec C_2$, that is, C_2 is accessible from C_1 (again, for the minimal chain), then we require that there be no class C' of states *outside* C with $C_1 \prec C' \prec C_2$: all paths leading from $i \in C_1$ to $j \in C_2$ must be wholly contained in C. (See Theorem 2 of [8] and the remarks at the end of Section 5 of that paper.)

(2) We call our invariance conditions the *Reuter FE conditions*, because they are G.E.H. Reuter's familiar necessary and sufficient conditions for the minimal transition function to be the unique solution to the forward equations when Q is not regular (see Section 6 of [16]); under our assumption that Q be regular, the Reuter FE conditions have no bearing on the forward equations.

Proof. Let m be a μ-invariant probability measure for Q. If the Reuter FE conditions hold, then any non-trivial, non-negative solution y to (2.4), for say $\nu = 1$, must satisfy $\sum_{i\in C} y_i = \infty$. However, since $\sum_{i\in C} m_i < \infty$, such a solution cannot satisfy $y_i \le m_i$ for all i. Thus, by Proposition 3, m is μ-invariant for P.

4 When absorption is not certain

When the absorption probabilities are less than 1 we cannot use Theorem 1 because, under the conditions we have imposed (specifically, the regularity of Q), the μ-invariant measure cannot be finite. To see this, first observe that if m is a finite μ-invariant measure for P with $\mu > 0$ then, for all $i \in C$,

$$\lim_{t\to\infty} \sum_{j\in C} p_{ij}(t) = 0,$$

since from (2.1) we have that

$$m_i p_{ij}(t) \le e^{-\mu t} m_j, \qquad j \in S.$$

But P is honest, and so the probability of absorption starting in i, given by

$$a_i = \lim_{t\to\infty} p_{i0}(t),$$

is equal to 1 for all $i \in C$.

When the absorption probabilities *are* less than 1, the natural premise is that the μ-invariant measure m be finite *with respect to* $a = (a_i,\ i \in S)$, that is, $\sum_{i\in C} m_i a_i < \infty$, and, as we shall see, the conditions of Theorem 1 can be relaxed accordingly. (Since m is the subject of our attention, we prefer this to the measure-theoretic statement that a is an m-measurable function.) The premise arises in connection with the more general definition of a quasistationary distribution:

Definition 2. Let $m = (m_j,\ j \in C)$ be a measure over C such that $\sum_{j\in C} m_j a_j < \infty$ and define $h(\cdot) = (h_j(\cdot),\ j \in S)$ by (2.3) and $p = (p_j,\ j \in C)$ by

$$p_j = \frac{m_j a_j}{\sum_{i\in C} m_i a_i}, \qquad j \in C.$$

Then, p is a *quasistationary distribution* if, for all $t > 0$ and $j \in C$,

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

Our next result, which is a generalization of Theorem 1, provides a means of determining quasistationary distributions directly from the q-matrix in cases where absorption occurs with probability less than 1.

Theorem 2. If the equations

$$\sum_{i\in C} y_i q_{ij} = \nu y_j, \quad j \in C, \tag{4.6}$$

have no non-trivial, non-negative solution such that $\sum_{i\in C} y_i a_i < \infty$, for some (and then all) $\nu > 0$, then all μ-invariant measures for Q which are finite with respect to a are also μ-invariant for P.

Proof. Suppose that the Reuter FE conditions (4.6) hold. Then, any non-trivial, non-negative solution to (2.4) satisfies $\sum_{i\in C} y_i a_i = \infty$. But, since $\sum_{i\in C} m_i a_i < \infty$, we cannot have $y_i \le m_i$ for every i and so, again by Proposition 3, m must be μ-invariant for P.

An alternative proof, which also provides a useful way of interpreting Theorem 2, is based on the dual of Q, namely the q-matrix $\bar{Q} = (\bar{q}_{ij},\ i,j \in S)$ given by

$$\bar{q}_{ij} = q_{ij} a_j / a_i, \qquad i,j \in S.$$

This dual q-matrix is *conservative* because $a = (a_j,\ j \in S)$ is an invariant vector for Q, and, by Lemma 3.3 (ii) of [9], the corresponding minimal transition function $\bar{P}$ bears the same duality relationship with P:

$$\bar{P}_{ij}(t) = P_{ij}(t) a_j / a_i, \qquad i,j \in S,\ t \ge 0.$$

Since a is an invariant vector for P, $\bar{P}$ is honest ($\bar{Q}$ regular) and is hence the unique $\bar{Q}$-transition function. Now, on setting $\bar{m}_j = m_j a_j$, $j \in C$, we see that m is μ-invariant for Q if and only if $\bar{m}$ is μ-invariant for $\bar{Q}$, and, that m is μ-invariant for P if and only if $\bar{m}$ is μ-invariant for $\bar{P}$. It is then a simple matter to check that Theorem 2 follows by applying Theorem 1 to $\bar{Q}$.

In applications involving chains for which absorption occurs with probability less than 1, it is frequently easier to construct the dual transition rates from the absorption probabilities and then apply Theorem 1. We shall use this approach in Section 5.

5 Birth and death processes

We shall illustrate the results of the previous section with reference to absorbing birth and death processes. Some further applications are described in [4].

Van Doorn [18] has given a complete treatment of questions concerning the existence of quasistationary distributions for absorbing birth and death processes in cases where the probability of absorption is 1. We shall explain how his conditions for the existence of quasistationary distributions arise in the context of Theorem 1 and then extend these results to cases where absorption occurs with probability less than 1.

An absorbing birth and death process on $S = \{0, 1, \ldots\}$ 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 $(\lambda_i,\ i \geq 0)$ and the death rates $(\mu_i,\ i \geq 0)$ satisfy $\lambda_i,\ \mu_i > 0$, for $i \geq 1$, and $\lambda_0 = \mu_0 = 0$. Thus, 0 is an absorbing state and $C = \{1, 2, \ldots\}$ is an irreducible class. We shall assume that

$$\sum_{i=1}^{\infty} \frac{1}{\lambda_i \pi_i} \sum_{j=1}^{i} \pi_j = \infty, \tag{5.7}$$

where $\pi_1 = 1$ and

$$\pi_i = \prod_{j=2}^{i} \frac{\lambda_{j-1}}{\mu_j}, \qquad i \geq 2,$$

a condition which is necessary and sufficient for Q to be regular (see Section 3.2 of [1]).

The classical Karlin and McGregor theory of birth and death processes involves the recursive construction of a sequence of orthogonal polynomials using the equations for an x-invariant vector (see [18]): define $(\phi_i(\cdot),\ i \in C)$, where $\phi_i : \mathrm{R} \to \mathrm{R}$, by $\phi_1(x) = 1$,

$$\lambda_1 \phi_2(x) = \lambda_1 + \mu_1 - x,$$

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

and let

$$m_i = \pi_i \phi_i(x), \qquad i \in C,\ x \in \mathrm{R}. \tag{5.8}$$

It can be shown [18] 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 [5]). Since Q is reversible with respect to π, that is,

$$\pi_i q_{ij} = \pi_j q_{ji}, \qquad i, j \in C, \tag{5.9}$$

it follows, from Theorem 4.1 b(ii) of [9], 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. Something which is not at all obvious, is that when the probability of absorption is 1, that is

$$A := \sum_{i=1}^{\infty} \frac{1}{\lambda_i \pi_i} = \infty, \tag{5.10}$$

as well as $\lambda > 0$, we have that $\sum_{i=1}^{\infty} \pi_i \phi_i(x) < \infty$ for all x in the range $0 < x \leq \lambda$ (see [3] and the proof of Theorem 3.2 of [18]). Thus, when $A = \infty$, each x-invariant measure for x in this range is finite, and so in order to apply Theorem 1 it remains only to check the Reuter FE conditions. (Note that $A = \infty$ implies (5.7) and hence the regularity of Q). It is well known (see Section 3.2 of [1]) that the Reuter FE conditions hold whenever

$$D := \sum_{i=1}^{\infty} \frac{1}{\lambda_i \pi_i} \sum_{j=i+1}^{\infty} \pi_j = \infty. \tag{5.11}$$

So, in the case where absorption occurs with probability 1, $D = \infty$ is sufficient to ensure that for every x in the range $0 < x \leq \lambda$, $m = (m_i,\ i \in C)$, given by $m_i = \pi_i \phi_i(x)$, is a (finite) x-invariant measure for P and, hence, can be normalized to produce a quasistationary distribution. Thus, we have proved the following result, which is encapsulated by Theorem 3.2 (i) of [18] (see also Theorem 3.5 (i) of [6]):

Theorem 3. Consider a birth and death process with $A = \infty$ (which of necessity is regular). Then, for every μ in the range $0 < \mu \leq \lambda$, the essentially unique μ-invariant measure m for Q is finite. Furthermore, if $D = \infty$, then m is always μ-invariant for P and $p = (p_j,\ j \in C)$, given by

$$p_j = \frac{\pi_j \phi_j(\mu)}{\sum_{i \in C} \pi_i \phi_i(\mu)}, \qquad j \in C,$$

is a quasistationary distribution.

Let us now deal with the case where absorption occurs with probability less than 1, that is, $A < \infty$. The absorption probabilities are given by $a_0 = 1$ and

$$a_j = \frac{\mu_1}{1 + \mu_1 A} \sum_{i=j}^{\infty} \frac{1}{\lambda_i \pi_i}, \qquad j \in C. \tag{5.12}$$

As suggested at the end of Section 4 we shall construct $\bar{Q}$, the dual of Q, and apply Theorem 1 to $\bar{Q}$. This is clearly the q-matrix of an absorbing birth and death process on S whose birth rates and death rates are given (in an obvious notation) by

$$\bar{\lambda}_j = \lambda_j a_{j+1}/a_j \quad \text{and} \quad \bar{\mu}_j = \mu_j a_{j-1}/a_j, \qquad j \in C,$$

with $\bar{\lambda}_0 = \bar{\mu}_0 = 0$. The corresponding potential coefficients are given by $\bar{\pi}_j = \pi_j a_j^2/a_1^2$, $j \in C$, and the polynomials by $\bar{\phi}_j = \phi_j a_1/a_j$, $j \in C$. It follows that $\bar{m} = (\bar{m}_j,\ j \in C)$, the essentially unique μ-invariant measure for $\bar{Q}$, is given by $\bar{m}_j = m_j a_j/a_1$, $j \in C$. It is easily shown that the counterparts, $\bar{A}$ and $\bar{D}$, of the series in (5.10) and (5.11) are both divergent. Hence $\bar{m}$ is finite and, by Theorem 1, $\bar{m}$ is μ-invariant for $\bar{P}$. We have therefore proved the following result, which can be compared with Theorem 3.5 (ii) of [6]:

Theorem 4. Consider a regular birth and death process with $A < \infty$. Then, for every μ in the range $0 < \mu \leq \lambda$, the essentially unique μ-invariant measure m for Q is finite with respect to a. Furthermore, m is always μ-invariant for P and $p = (p_j,\ j \in C)$, given by

$$p_j = \frac{\pi_j \phi_j(\mu) a_j}{\sum_{i \in C} \pi_i \phi_i(\mu) a_i}, \qquad j \in C,$$

is a quasistationary distribution.

Remark. What has happened to the invariance condition $D = \infty$? This condition is not needed when $A < \infty$, for it is the regularity of Q which is making the result work. Indeed, in a more general setting, where Q is not regular and our attention is focused on the minimal transition function, we can show that if $A < \infty$, then $\bar{D} = \infty$ if and only if the series in (5.7) diverges. It is also worth remarking that, in this more general context, Theorem 3 remains valid with P being interpreted as the minimal process.

6 Some concluding remarks

We have already noted that the transition rates of a birth and death process are *reversible* with respect to a measure π. Since the Reuter FE conditions are expressed simply and explicitly in terms of the divergence of certain series, one might expect a simplification of the Reuter FE conditions in the general case of reversible Markov chains. We shall content ourselves with the following simple result:

Theorem 5. Suppose that there exists a collection of positive numbers $\pi = (\pi_i,\ i \in S)$ satisfying (5.9). Then, every μ-invariant measure $m = (m_i,\ i \in C)$ for Q satisfying $\sup_{i \in C}\{m_i/\pi_i\} < \infty$ is μ-invariant for P.

Remarks. (1) Neither π nor m need be finite. We require only that m be bounded above by π.

(2) Our assumption that Q be regular cannot be relaxed.

Proof. Let m be a μ-invariant measure which is bounded above by π and suppose that m *is not* μ-invariant for P. Then, by Proposition 3, the equations (2.4) have a non-trivial solution y, certainly for $\nu > 0$. On substituting (5.9) into (2.4) we find that $z = (z_j,\ j \in C)$, given by $z_j = y_j/\pi_j$, satisfies

$$\sum_{i \in C} q_{ji} z_i = \nu z_j, \tag{6.13}$$

with $0 < z_j \le m_j/\pi_j$, $j \in C$. But, $\sup_{i \in C}\{m_i/\pi_i\} < \infty$, and so we have found a bounded, non-trivial, non-negative solution to (6.13), which, by Theorem 2.2.7 of [1], contradicts our assumption that Q is regular.

We shall conclude with a tantalizing conjecture. For a birth and death process with absorption probability 1, Theorem 3 identifies a one-parameter family of quasistationary distributions under the condition that $D = \infty$. As mentioned earlier, this result is contained in the first part of Theorem 3.2 of [18]. The second part of van Doorn's result states that if $D < \infty$, then there is *only one* quasistationary distribution: in the notation of Theorem 3, if $D < \infty$, then m is μ-invariant for P only when $\mu = \lambda$, and $p = (p_j,\ j \in C)$, given by

$$p_j = \frac{\pi_j \phi_j(\lambda)}{\sum_{i \in C} \pi_i \phi_i(\lambda)}, \qquad j \in C,$$

is the only quasistationary distribution.

Since, for birth and death processes, the Reuter FE conditions hold whenever the D series (5.11) diverges, we arrive at the following conjecture, which would extend Theorems 1 and 2:

Conjecture. If the Reuter FE conditions fail, that is, the equations

$$\sum_{i \in C} y_i q_{ij} = \nu y_j, \quad j \in C, \tag{6.14}$$

have a non-trivial, non-negative solution satisfying $\sum_{i \in C} y_i a_i < \infty$, for some (and then all) $\nu > 0$, then μ-invariant probability measures for Q which are finite with respect to a are μ-invariant for P *only* when μ is the decay parameter of C.

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