RECENT ADVANCES IN THE THEORY AND APPLICATION OF QUASISTATIONARY DISTRIBUTIONS

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Abstract. There are many stochastic systems arising in areas as diverse as wildlife management, chemical kinetics and reliability theory, which eventually "die out", yet appear to be stationary over any reasonable time scale. The notion of a *quasistationary distribution* has proved to be a potent tool in modelling this behaviour. In finite-state systems the existence of a quasistationary distribution is guaranteed. However, in the infinite-state case this may not always be so, and the question of whether or not quasistationary distributions exist requires delicate mathematical analysis. The purpose of this paper is to present simple conditions for the existence of quasistationary distributions for continuous-time Markov chains and to demonstrate how these can be applied in practice.

1. Introduction

Quasistationary distributions have been used in a variety of diverse contexts for modelling the long-term behaviour of stochastic systems which, in some sense, terminate, but appear to be stationary over any reasonable time scale. For example, in the context of modelling chemical reaction kinetics, there are a number of reactions in which one or more species can become depleted, yet these reactions settle down quickly to a stable equilibrium; quasistationary distributions have been used here to model the concentration of the catalyst in reactions in which the catalyst can become exhausted (see, for example, Oppenheim et al. (1977), Turner and Malek-Mansour (1978), Dambrine and Moreau (1981a, 1981b), Parsons and Pollett (1987) and Pollett (1988b)). In the context of reliability theory, one might wish to determine the distribution of the residual lifetime of a system at some arbitrary time t, conditional on the system being functional (see, for example, Kalpakam and Shahul Hameed (1983), Pijnenburg and Ravichandran (1990) and Pijnenburg et al. (1990)); in the case of a two-unit warm-standby redundant system, the limiting form of this conditional distribution, as t becomes large, is always exponential, no matter what the distribution of lifetimes and repair times (Kalpakam and Shahul Hameed (1983)). Yet another example of the use of quasistationary distributions is in the area of wildlife

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management, where these have proved to be a potent tool in predicting persistence times, and the distribution of the number of individuals, in animal populations which are subject to large-scale mortality or emigration; in spite of the fact that the usual stochastic models predict eventual extinction, these populations can be surprisingly resilient (see, for example, Scheffer (1951), Mech (1966), Klein (1968), Holling (1973), Pakes (1987), Pollett (1987), and Pakes and Pollett (1989)).

The idea of a quasistationary distribution can be traced back to the work of the Russian Mathematician A.M. Yaglom, who showed that the limiting conditional distribution of the number in the n^{th} generation of the Galton Watson branching process always exists in the subcritical case (see Yaglom (1947)). But, it was not until the early sixties, and largely stimulated by the remarkable work of Vere-Jones (1962), and later Kingman (1963), that a general theory was annunciated. Since then, there have been a number of significant advances on questions concerned with the existence of quasistationary distributions; in the present context of continuous-time Markov chains, see, for example, Darroch and Seneta (1967), Good (1968), Vere-Jones (1969), Flaspohler (1974), Tweedie (1974), Cavender (1978), van Doorn (1991), Kijima and Seneta (1991), Kijima (1992) and van Doorn and Kijima (1992) (a spectacularly clear account of much of this work is also given in the recent text by Anderson (1991)).

In this paper I shall give a unified account of the theory of quasistationary distributions for continuous-time Markov chains. Simple conditions will be established for the existence of quasistationary distributions and these will be illustrated with reference to finite-state systems, birth and death processes, and the birth, death and catastrophe process.

2. The existence of quasistationary distributions

We shall suppose that the system in question can be modelled as a time-homogeneous Markov chain, $(X(t),\ t \geq 0)$, taking values in a discrete set S. Let $Q = (q_{ij},\ i,j \in S)$ be the q-matrix of the chain (assumed to be stable and conservative), so that $q_{ij}\ (\geq 0)$, for $j \neq i$, represents the transition rate from state i to state j and $q_{ii} = -q_i$, where $q_i = \sum_{j \neq i} q_{ij}\ (< \infty)$ represents the transition rate out of state i. In addition, we shall suppose that Q is regular, so that $X(\cdot)$ is the unique chain with these rates. Checking for regularity should be, though apparently seldom is, a part of the routine of modelling. Simple sufficient conditions for the regularity of Q are contained in Pollett and Taylor (1993). The condition $\sup_j q_j < \infty$, which is predominant in the engineering literature, is certainly too strong for practical purposes; for example, it rules out branching and catastrophe processes and random delay systems.

We shall be concerned with evanescent chains, so, for simplicity, let us take 0 to be the sole absorbing state, that is, $q_0 = 0$, and suppose that $S = \{0\} \cup C$, where $C = \{1, 2, \dots\}$ is an irreducible transient class. In order that there be a positive probability of reaching 0, given that the chain starts in C, we shall suppose that $q_{i0} > 0$ for at least one $i \in C$.

The definition of a quasistationary distribution, which I shall use here, is the one introduced by van Doorn (1991). Let $P(\cdot) = (p_{ij}(\cdot),\ i,j \in S)$ be the transition function of the chain, so that $p_{ij}(t) = \Pr(X(t) = j | X(0) = i)$, for $t \geq 0$.

Definition. *Let $m = (m_j,\ j \in C)$ be a probability distribution over C and let $p_j(t) =$*

$\sum_{i\in C} m_i p_{ij}(t)$, for $j \in S$ and $t \geq 0$. Then, m is a quasistationary distribution if, for all $t > 0$ and $j \in C$, $p_j(t)/(\sum_{i\in C} p_i(t)) = m_j$. 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:

Proposition 1 (Nair and Pollett (1993))**.** *Let $m = (m_j,\ j \in C)$ be a probability distribution over C. Then, m is a quasistationary distribution if and only if, for some $\mu > 0$, m is μ-invariant on C for P, that is*

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

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 (1) as

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

and then divide by t and let $t \downarrow 0$. Proceeding formally, we get

$$\sum_{i\in C:\, i\neq j} m_i q_{ij} = (q_j - \mu) m_j, \qquad j \in C, \tag{2}$$

or, equivalently,

$$\sum_{i\in C} m_i q_{ij} = -\mu m_j, \qquad j \in C. \tag{3}$$

Accordingly, we shall say that m is *μ-invariant on C for Q* whenever (3) holds. The above argument can be justified rigorously (see Proposition 2 of Tweedie (1974)), and so, in view of Proposition 1, we have the following result:

Proposition 2. *If m is a quasistationary distribution then, for some $\mu > 0$, m is μ-invariant on C for Q.*

The more interesting question of when a positive solution, m, to (3) is also a solution to (1) was answered in Pollett (1986, 1988a). However, the necessary and sufficient conditions obtained are usually difficult to verify in practice. If we take into account the fact that, for m to be a quasistationary distribution, one requires $\sum_{j\in C} m_j = 1$, then much simpler conditions obtain, as our next result demonstrates. It can be deduced from Theorems 3.2, 3.4 and 4.1 of Nair and Pollett (1993); the assumption made here, that Q be regular, facilitates the simpler and more direct proof given below.

Proposition 3. *Let $m = (m_j,\ j \in C)$ be a probability distribution over C and suppose that m is μ-invariant on C for Q. Then,*

$$\mu \le \sum_{j \in C} m_j q_{j0}, \tag{4}$$

with equality if and only if m is a quasistationary distribution.

Proof. First observe that, since m is a probability distribution, there exists a $j \in C$ such that $m_j > 0$. Hence, because m is μ-invariant on C for Q and C is irreducible, we have, from (2), that $\mu \le \inf_{j \in C} q_j$ and that $m_j > 0$ for *all* $j \in C$.

Define $Q^* = (q^*_{ij},\ i,j \in C)$ by $q^*_{ij} = m_j q_{ji}/m_i$, for $j \ne i$, and $q^*_{ii} = -q^*_i$, where $q^*_i = q_i - \mu$. Clearly $q^*_{ij} \ge 0$ for all $j \ne i$ and $0 \le q^*_i < \infty$. And, since m is μ-invariant on C for Q, we have that $\sum_{j \in C} q^*_{ij} = 0$. Thus, Q^* is a stable and conservative q-matrix over C (Q^* is called the μ-reverse of Q with respect to m). Let $P^*(\cdot) = (p^*_{ij}(\cdot),\ i,j \in C)$ be the transition function of the minimal process associated with Q^*. Then, by Lemma 3.3 of Pollett (1988a), we have that

$$m_i p_{ij}(t) = e^{-\mu t} m_j p^*_{ji}(t), \qquad i,j \in C. \tag{5}$$

Summing this equation over $j \in C$, and remembering that, because Q is regular, $\sum_{j \in S} p_{ij}(t) = 1$, we get

$$m_i(1 - p_{i0}(t)) = e^{-\mu t} \sum_{j \in C} m_j p^*_{ji}(t), \qquad i \in C.$$

On summing *this* equation over i, and using Fubini's theorem, we find that

$$\sum_{i \in C} m_i p_{i0}(t) = 1 - e^{-\mu t} \sum_{j \in C} m_j \sum_{i \in C} p^*_{ji}(t),$$

or, equivalently,

$$\sum_{i \in C} m_i p_{i0}(t) = 1 - e^{-\mu t} + e^{-\mu t} \sum_{j \in C} m_j d^*_j(t), \tag{6}$$

where $d^*_i(t) = 1 - \sum_{j \in C} p^*_{ij}(t)$. Notice that $d^*_i(t) \ge 0$, since, because P^* is a transition function, we have that $\sum_{j \in C} p^*_{ij}(t) \le 1$, for all $i \in C$ and $t \ge 0$.

Now, since P satisfies the forward differential equations, we have, in particular, that

$$p'_{i0}(t) = \sum_{j \in C} p_{ij}(t) q_{j0}, \qquad i \in C,\ t > 0,$$

or, equivalently,

$$p_{i0}(t) = \sum_{j \in C} \int_0^t p_{ij}(s) q_{j0}\, ds, \qquad i \in C,\ t > 0.$$

Multiplying by m_i and summing over $i \in C$, and then using (5) once again, we get

$$\begin{aligned}\sum_{i\in C} m_i p_{i0}(t) &= \int_0^t \sum_{j\in C}\sum_{i\in C} m_i p_{ij}(s) q_{j0}\,ds \\ &= \int_0^t e^{-\mu s}\sum_{j\in C} m_j \sum_{i\in C} p^*_{ji}(s) q_{j0}\,ds \\ &= \int_0^t e^{-\mu s}\sum_{j\in C} m_j (1-d^*_j(s)) q_{j0}\,ds \\ &= \int_0^t e^{-\mu s}\left(\sum_{j\in C} m_j q_{j0} - \sum_{j\in C} m_j d^*_j(s) q_{j0}\right) ds \\ &= \frac{1}{\mu}(1-e^{-\mu t})\sum_{j\in C} m_j q_{j0} - \int_0^t e^{-\mu s}\sum_{j\in C} m_j d^*_j(s) q_{j0}\,ds.\end{aligned}$$

On combining this equation with (6) we find that

$$\mu e^{-\mu t}\sum_{j\in C} m_j d^*_j(t) + \int_0^t \mu e^{-\mu s}\sum_{j\in C} m_j d^*_j(s) q_{j0}\,ds = (1-e^{-\mu t})\left(\sum_{j\in C} m_j q_{j0} - \mu\right).$$

The left-hand side of this equation is always non-negative, and so we deduce that (4) must hold. It is also clear that d^*_i is identically 0 for each i if and only if $\mu = \sum_{j\in C} m_j q_{j0}$. But, from (5), we have that

$$\sum_{i\in C} m_i p_{ij}(t) = e^{-\mu t} m_j (1-d^*_j(t)), \qquad j \in C,$$

and so a necessary and sufficient condition for m to be μ-invariant on C for P is that $d^*_i(t) = 0$, for all $i \in C$ and $t \geq 0$. Thus, in view of Proposition 1, we have proved that m is a quasistationary distribution if and only if equality holds in (4).

Proposition 3 corrects Theorem 6 of Vere-Jones (1969) and the first part of Corollary 1 of Pollett (1986), both of which assert falsely that a μ-invariant probability distribution on C for Q is *always* μ-invariant of C for P. The error was pointed out by van Doorn (1991) and the counter example which he presented provides the basis for the arguments used above. In determining where the error occurred in the original proof, Vere-Jones and I were able to identify a simple sufficient condition (see Corollary 2 of Pollett and Vere-Jones (1992)). It is instructive to see how this condition arises in the context of Proposition 3. Consider the following formal argument, based on summing (3) over $j \in C$:

$$\sum_{i\in C} m_i q_{i0} = -\sum_{i\in C} m_i \sum_{j\in C} q_{ij} = -\sum_{j\in C}\sum_{i\in C} m_i q_{ij} = \mu \sum_{j\in C} m_j = \mu. \tag{7}$$

The interchange of summation is not permitted in general, but can be justified under various conditions (see Section 3.7 of Knopp (1956)). For example, the interchange is permitted if the double sum in (7) is absolutely convergent, and a necessary and sufficient condition for this is $\sum_{j\in C} m_j q_j < \infty$. Thus, we have the following result:

Corollary 1. *Let $m = (m_j,\ j \in C)$ be a probability distribution over C and suppose that m is μ-invariant on C for Q. Then, if $\sum_{j\in C} m_j q_j < \infty$, m is a quasistationary distribution and $\mu = \sum_{j\in C} m_j q_{j0}$.*

3. Applications

Finite-state systems. If S is a finite set, then clearly $\sum_{j\in C} m_j q_j < \infty$ and so every μ-invariant probability distribution on C for Q is a quasistationary distribution. Indeed, classical matrix theory can be used to show that the q-matrix restricted to C has eigenvalues with negative real parts, that $-\mu$ is the dominant eigenvalue (it has maximal real part), that this eigenvalue always has multiplicity 1, and, that both the corresponding left and right eigenvectors have positive entries (see Mandl (1960), and Darroch and Seneta (1967)); the left eigenvector is, of course, the quasistationary distribution. Thus, for example, in Markovian reliability models, the stationary conditional distribution of the number of functioning units (conditional on the system not having failed) can be obtained as the dominant left eigenvector of the transition-rate matrix restricted to the transient states. In most cases one is forced to evaluate the dominant eigenvector numerically. If the number of states is reasonably small, say 100, then one can use any of the standard methods (inverse iteration, for example) which are widely available as part of matrix packages, such as MATLAB. If the number of states is even moderately large, these methods are ineffective, both in respect of storage and CPU time. For example, if there are 10^4 states, Q requires 400 Mbytes of storage. If Q is sparse, or if it possesses a banded structure that can be usefully exploited, then moderately large systems can be handled without difficulty. Pollett and Stewart (1994) have developed an iterative version of Arnoldi's algorithm (see, for example, Golub and van Loan (1989)) for dealing with sparse q-matrices, and this has been used to evaluate the quasistationary distribution, to within a tolerance of 10^{-6}, for a variety of systems, with of the order of 10^4 states, in times ranging from 15 to 30 CPU minutes on a Sun SPARC 2. If the number of states is very large, say 10^8, then it is frequently the case that deterministic approximations (see, for example, Pollett and Roberts (1990)) or diffusion approximations (see, for example, Parsons and Pollett (1987), Pollett (1990, 1992), Pollett and Vassallo (1992), and Pollett and Stewart (1994)) can be used to provide accurate estimates of the quasistationary distribution.

Birth and death processes. These are widely used in modelling stochastic systems which arise in engineering, the information sciences and biology. Van Doorn (1991) has given a complete treatment of questions concerning the existence of quasistationary distributions for absorbing birth and death processes in cases when the probability of absorption is 1. I shall explain how his conditions for the existence of quasistationary distributions arise in the context of Proposition 3. The q-matrix of an absorbing birth and death process is of the form

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

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 $C = \{1, 2, \dots\}$ is an irreducible class.

The classical Karlin and McGregor theory of birth and death processes involves the recursive construction of a sequence of orthogonal polynomials (see van Doorn (1991)). Define $(\phi_i(\cdot),\ i \geq 1)$, where $\phi_i : \mathrm{R} \to \mathrm{R}$, by $\phi_1(x) = 1$,

$$\lambda_1\phi_2(x) = \lambda_1 + \mu_1 - x,$$
$$\lambda_i\phi_{i+1}(x) - (\lambda_i + \mu_i)\phi_i(x) + \mu_i\phi_{i-1}(x) = -x\phi_i(x), \qquad i \geq 2.$$

Now define $\pi = (\pi_i,\ i \geq 1)$ by $\pi_1 = 1$ and $\pi_i = \prod_{j=2}^{i} \lambda_{j-1}/\mu_j$, for $i \geq 2$, and let $m_i = \pi_i\phi_i(x)$. It can be shown (van Doorn (1991)) that $\phi_i(x) > 0$ for x in the range $0 \leq x \leq \lambda$, where $\lambda\ (\geq 0)$ is the decay parameter of C (see Kingman (1963)). Since π is a subinvariant measure for Q, that is $\sum_{i\in S} \pi_i q_{ij} \leq 0$, it follows, from Theorem 4.1 b(ii) of Pollett (1988), that, for each fixed x in the above range, $m = (m_i,\ i \geq 1)$ is an x-invariant measure on C for Q, that is, m satisfies (3) with $\mu = x$. Indeed, m is uniquely determined up to constant multiples. Proposition 3 tells us that if m can be normalized to produce a proper distribution on C, that is, if $\sum_{i=1}^{\infty} \pi_i\phi_i(x) < \infty$, then the normalized m will be a quasistationary distribution if and only if

$$\sum_{i=1}^{\infty} r_i(x) = 1, \tag{8}$$

where $r_i(x) = \mu_1^{-1}\pi_i x\phi_i(x)$, a conclusion reached by van Doorn using direct methods. Van Doorn's Theorem 3.2 can then be used to determine all the values of x for which (8) holds, at least under the condition

$$\sum_{i=1}^{\infty} \frac{1}{\lambda_i\pi_i} = \infty, \tag{9}$$

which ensures, not only that Q is regular, but that absorption occurs with probability 1. If, in addition, the series

$$\sum_{i=1}^{\infty} \frac{1}{\lambda_i\pi_i} \sum_{j=i+1}^{\infty} \pi_j \tag{10}$$

diverges then (8) holds for *all* x in $(0, \lambda]$, while if it converges then (8) holds if and only if $x = \lambda$. Proposition 3 then tells us that, in either case, $r(x) = (r_i(x),\ i \geq 1)$ is a quasistationary distribution. Indeed, because m is uniquely determined for each x, *all* quasistationary distributions have been obtained under (9); if the series (10) converges, then there is only one, namely $r(\lambda)$, while if (10) diverges, $(r(x),\ 0 < x \leq \lambda)$ comprises a one-parameter family of quasistationary distributions.

The birth, death and catastrophe process. The introduction of a catastrophe component allows greater flexibility in modelling. The q-matrix of the birth, death and catastrophe process is given by

$$\begin{aligned} q_{i,i+1} &= aq_i, && i \geq 0, \\ q_{i,i} &= -q_i, && i \geq 0, \\ q_{i,i-k} &= q_i b_k, && i \geq 2,\ k = 1, 2 \dots i-1, \\ q_{i,0} &= q_i \sum_{k=i}^{\infty} b_k, && i \geq 1, \end{aligned}$$

where $q_0 = 0$, $q_i > 0$, for $i \geq 1$, $a > 0$, $b_i > 0$ for at least one value of $i \geq 1$ and $a + \sum_{i=1}^{\infty} b_i = 1$. Thus, at a jump time, a birth occurs with probability a, or otherwise a catastrophe occurs, the size of which is determined by the probabilities b_i, $i \geq 1$. Clearly, 0 is an absorbing state and $C = \{1, 2, \dots\}$ is an irreducible class. It is usual to set $q_i = \rho i$, where $\rho > 0$, so that jumps occur at a constant "per capita" rate ρ. Notice that if, of the b_i's, only b_1 is positive, then we recover the simple linear birth and death process. It is well known, and easy to prove (see, for example, Pakes (1987)), that the probability of absorption, starting in state i, is 1 if and only if D, given by

$$D = a - \sum_{i \in C} i b_i = 1 - \sum_{i \in C} (i+1) b_i,$$

is less than or equal to 0. D can be thought of as the drift, and, accordingly, the process is said to be subcritical, critical or supercritical according as D is negative, zero or positive. In a way that is analogous to the theory of Markov branching processes (see for example, Athreya and Ney (1972)), an important role is played by the probability generating function, f, given by

$$f(s) = a + \sum_{i \in C} b_i s^{i+1}, \qquad |s| < 1,$$

and the related function, b, given by $b(s) = f(s) - s$. In identifying the quasistationary distribution, we shall need the following facts from branching process theory: that b is convex on $[0, 1]$, that $b(s) = 0$ has a unique solution, σ, on this interval, that $\sigma = 1$ or $0 < \sigma < 1$ according as $D \geq 0$ or $D < 0$, and, that $b(s) \geq 0$ on $[0, \sigma]$.

On substituting the transition rates in equation (3), we get

$$-(\rho - \mu) m_1 + \sum_{k=2}^{\infty} k \rho b_{k-1} m_k = 0,$$

$$(j-1) \rho a m_{j-1} - (j\rho - \mu) m_j + \sum_{k=j+1}^{\infty} k \rho b_{k-j} m_k = 0, \qquad j \geq 2.$$

If we try a solution of the form $m_j = t^j$, the first equation tells us that $\mu = -\rho b'(t)$, of necessity, and, on substituting both of *these* quantities in the second equation, we find that $b(t) = 0$. Hence, we may set $t = \sigma$, thus providing a positive solution, $m = (m_j,\ j \in C)$, to (3), such that $\sum_{j \in C} m_j < \infty$ whenever $\sigma < 1$. Under this latter condition, we also have $\sum_{j \in C} m_j q_j = \sum_{j \in C} \sigma^j j \rho < \infty$. Thus, by Corollary 1, we have the following result, which is implicit in the proof of Theorem 5.1 of Pakes (1987):

Proposition 4. *The subcritical linear birth, death and catastrophe process has a geometric quasistationary distribution, $m = (m_j,\ j \in C)$, given by*

$$m_j = (1-\sigma)\sigma^{j-1}, \qquad j \in C,$$

where σ is the unique solution to $b(s) = 0$ on the interval $[0, 1]$.

Computational methods for infinite-state systems. If the quasistationary distribution cannot be exhibited explicitly, or if the form of the quasistationary distribution is not amenable to numerical evaluation, one is forced to use a direct computational approach. One widely used method is to truncate the restricted q-matrix to an $n \times n$ matrix, $Q^{(n)}$, and construct a sequence, $\{m^{(n)}\}$, such that $m^{(n)}$ is the left-eigenvector of $Q^{(n)}$ associated with the eigenvalue with maximum real part. Then, one estimates the quasistationary distribution by taking successively larger truncations until the difference in the normalized eigenvectors is as small as desired. For a detailed account of these procedures, see Seneta (1973) and Tweedie (1973). When this approach is used, the iterative Arnoldi method, referred to above, often provides an efficient means of determining the sequence $\{m^{(n)}\}$.

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