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On the Problem of Evaluating Quasistationary Distributions for Open Reaction Schemes

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A number of recent papers have been concerned with the stochastic modeling of autocatalytic reactions. In some instances the birth and death model has been criticized for its apparent inadequacy in being able to describe the long-term behavior of the catalyst, in particular the fluctuations in the concentration of the catalyst about its macroscopically stable state. This criticism has been answered, to some extent, with the introduction of the notion of a quasistationary distribution; a number of authors have established the existence of limiting conditional distributions that can adequately describe these fluctuations. However, much of the work appears only to be appropriate for dealing with closed systems, for attention is usually restricted to finite-state birth and death processes. For open systems it is more appropriate to consider infinite-state processes and, from the point of view of establishing conditions for the existence of quasistationary distributions, extending the results for closed systems is far from straightforward. Here, simple conditions are given for the existence of quasistationary distributions for Markov processes with a denumerable infinity of states. These can be applied to any open autocatalytic system. The results also extend to explosive processes and to processes that terminate with probability less than 1.

KEY WORDS: Stochastic processes; quasistationary distributions; chemical kinetics.

1. INTRODUCTION

A number of authors have considered stochastic models for chemical reactions that terminate with the exhaustion of a particular species. Reactions involving autocatalysis comprise an important class of these and have been

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studied extensively. Two common examples that have been considered are[1-6]

$$\begin{aligned} A + X &\xrightarrow{k_1} 2X \\ 2X &\xrightarrow{k_2} B \end{aligned} \tag{1}$$

and[6-10]

$$\begin{aligned} A + X &\underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} 2X \\ X &\xrightarrow{k_2} B \end{aligned} \tag{2}$$

each system being open with respect to both A and B. It is clear that any stochastic model which properly accounts for the microscopic behavior of either reaction will predict eventual exhaustion of (the catalyst) X, unless, exceptionally, the quantity of X grows unboundedly. On the other hand, the usual deterministic models predict two stationary states, one unstable, corresponding to depletion of X, and the other stable. These models help to explain the apparent stationarity exhibited by the reactions, for they predict that after a relatively short time the system relaxes to the stable state, and then, after a very much longer period, it evanesces.[6,8,11] However, they do not provide information regarding the fluctuations about the stable state. These fluctuations can be adequately described, using a stochastic formulation, by considering *quasistationary distributions* and several authors have adopted this approach.[6,8-11] Oppenheim *et al.*[8] and Dambrine and Moreau[9,10] base their analysis on a finite-state birth and death model, but this appears to be appropriate only when the system in question is closed. Their assumption, that the process has a finite collection of possible states, ensures that quasistationary distributions always exist and that these can be determined from the right and left eigenvectors of the matrix of transition rates (truncated appropriately) corresponding to the eigenvalue with maximum real part.

For an infinite-state process, one that is appropriate for modeling open reaction systems, the situation is considerably more complicated. First, the transition rate matrix need not necessarily possess finitely many eigenvalues. Indeed, they may comprise a continuum, and positive eigenvectors can be obtained for a range of eigenvalues that is, at best, a finite closed interval. It might also be the case that the matrix possesses no positive eigenvectors, and, even when it does, it might not be possible to determine whether or not quasistationary distributions exist. Thus, the progression from a finite-state model to an infinite-state one is far from straightforward. The purpose of this paper is to provide conditions for the existence of quasistationary distributions for a continuous-time countable-state Markov process that are expressed solely in terms of its transition rates. Parsons and Pollett[6] used a more stringent set of conditions in obtaining quasistationary distributions for reaction system (1). However, these are inappropriate when dealing with processes that terminate with probability less than 1. The conditions I provide are quite adequate for dealing with this case. Further, there is no need to assume that the process is regular, that is, nonexplosive. It might be that termination is caused by the process performing infinitely many transitions in a finite time. Thus, the present conditions can be used to provide quasistationary distributions for explosive processes.

I study two types of quasistationary distribution, each of which involves conditioning on the event that the process does not terminate, or will not terminate in the distant future. This is related to the approach of Gaveau and Schulman[22] (see also Greensite and Halperin[23] and McGraw and Schulman[24]), whereby the process is conditioned on not exceeding a given level at any time in a specified interval. They consider the limit behavior as the length the time interval, and then the level, tend to infinity.

2. PRELIMINARIES

Consider a standard time-homogeneous Markov process $(X(t), t \geqslant 0)$ taking values in a countable state space S, with a stable conservative q-matrix of transition rates, that is, a collection $\mathsf{Q} = (q_{jk}, j, k \in S)$ of real numbers satisfying

$$0 \leqslant q_{jk} < \infty, \qquad k \neq j, \quad j, k \in S$$

$$0 \leqslant -q_{jj} \triangleq q_j < \infty, \qquad j \in S$$

$$\sum_{k \in S} q_{jk} = 0, \qquad j \in S$$

The quantity q_{jk} is the rate of the process from state j to state k and q_j is the total rate out of state j. Of course there are many processes with this set of transition rates. I shall suppose that $(X(t), t \geqslant 0)$ is the *minimal process*, the one whose transition probabilities $\mathsf{P}_t = (p_{jk}(t), j, k \in S)$ are the minimal solution to the backward differential equations.[12] This process may *explode* by performing infinitely many transitions in a finite time, since, for some collection of starting states, the times spent in successive states form a sequence of random variables whose sum T might well be finite. The transition probabilities admit the following interpretation:

$$p_{jk}(t) = P\{X(t) = k, t < T \mid X(0) = j\}, \qquad j, k \in S, \quad t \geqslant 0 \tag{3}$$

that is, $p_{jk}(t)$ is the probability that the process is in state k at time t after having performed at most a finite number of transitions starting in state j. It follows that

$$P\{T \leqslant t \mid X(0) = j\} = 1 - \sum_{k \in S} p_{jk}(t), \qquad j \in S$$

and so the process is *regular*, that is, nonexplosive, if and only if e_j, given by

$$e_j = 1 - \lim_{t \to \infty} \sum_{k \in S} p_{jk}(t)$$

the probability that the process explodes starting in state j, is equal to 0 for each j in S. It can be shown[12] that this is equivalent to stipulating that the equations

$$\sum_{k \in S} q_{jk} \xi_k = \nu \xi_j, \qquad j \in S$$

possess no bounded, nontrivial, nonnegative solution ξ for some (and then for all) $\nu > 0$. It is often difficult to verify the existence or otherwise of such a solution. However, S finite or $\{q_j, j \in S\}$ bounded is a sufficient condition for regularity.

3. QUASISTATIONARY DISTRIBUTIONS

The fact that the minimal process may explode gives rise to the possibility that some degree of quasistationarity might be evident, particularly in the case when explosion is not a certainty or if the time to explosion is rather long. In the case where $(X(t), t \geqslant 0)$ is not regular it is of interest, therefore, to determine if and under what conditions the usual limiting conditional distributions exist. These are

$$\lim_{t \to \infty} P\{X(t) = j \mid X(0) = i, A_t, B\}, \qquad i, j \in S \tag{4}$$

and

$$\lim_{t \to \infty} \lim_{s \to \infty} P\{X(t) = j \mid X(0) = i, A_{t+s}, B\}, \qquad i, j \in S \tag{5}$$

where $A_t = \{t < T\}$ is the event that the process has not exploded by time t and $B = \{T < \infty\}$ is the event that the process will eventually explode. Thus I seek the limiting probability of being in state j given that the process has not terminated or [in the case of (5)] will not terminate in the distant future, but that eventually it will. I condition on B to deal with the possibility that $P(B)$ might be less than 1.

Quasistationary distributions most commonly arise in connection with absorbing processes where they are used to describe the long-term behavior of the process before absorption occurs. In particular, limits of the form (4) and (5) are usually considered, but with A_t being the event that the process has not been absorbed by time t and B the event that it eventually will be. With little extra effort one can deal with processes that can terminate either by explosion *or* absorption. For simplicity, suppose that S consists of an irreducible (transient) class C and an absorbing state 0. Write

$$A_t = \{t < T \text{ and } X(t) \in C\}$$

and

$$B = \{T < \infty \text{ or } X(t) = 0 \text{ eventually}\}$$

with the understanding that α_k, given by

$$\alpha_k = P\{B \mid X(0) = k\}$$

is positive for some (and then for all) k in C.

The conditions for the existence of quasistationary distributions involve the solutions of the eigenvector equations

$$\sum_{k \in C} m_k q_{kj} = -\mu m_j, \qquad j \in C \tag{6}$$

and

$$\sum_{k \in C} q_{jk} x_k = -\mu x_j, \qquad j \in C \tag{7}$$

where μ is real and nonnegative. If C is a finite set of states, then one can always find *positive* solutions $\mathsf{m} = (m_j, j \in C)$ and $\mathsf{x} = (x_j, j \in C)$ for some $\mu \geqslant 0$, for the q-matrix truncated to C possesses an eigenvalue, say $-\lambda$, with maximal real part which is real and negative, and, corresponding to it, there are unique positive left and right eigenvectors m and x.[13] Further, the limits (4) and (5) always exist and define proper probability distributions over C that do not depend on the initial state i; the first is given by

$$m_j \Big/ \sum_{k \in C} m_k, \qquad j \in C \tag{8}$$

and the second by

$$m_j x_j \Big/ \sum_{k \in C} m_k x_k, \qquad j \in C \tag{9}$$

Note that since C is finite, the process cannot explode in C, and further assuming, as we must, that exit from C is possible, the process must eventually be absorbed. If C is infinite, then the existence of quasistationary distributions is not guaranteed. First, it may not be possible to find positive solutions to (6) and (7) for any $\mu \geqslant 0$, and, even when it is possible, the solutions for a given μ might not be unique. However, one can always find positive solutions to the corresponding systems of inequalities

$$\sum_{k \in C} m_k q_{kj} \leqslant -\mu m_j, \qquad j \in C \tag{10}$$

and

$$\sum_{k \in C} q_{jk} x_k \leqslant -\mu x_j, \qquad j \in C \tag{11}$$

This is possible for all $\mu \geqslant 0$ up to some finite value λ, known as the decay parameter, a quantity that plays a fundamental role in the theory of non-stationary processes. Indeed I have shown[14] that positive solutions m and x exist *if and only if* $0 \leqslant \mu \leqslant \lambda$. These solutions are said to be μ-subinvariant on C for Q, and μ-invariant if equality holds for all j in C. I have also obtained[15] necessary and sufficient conditions for μ-subinvariant quantities to be μ-invariant. However, these conditions are usually difficult to verify in practice and so, in order to simplify matters, I henceforth assume that (6) and (7) possess positive solutions for at least one value of $\mu \geqslant 0$. If no such solution exists, then certainly there can be no quasistationary distributions. Denote by m and x the solutions corresponding to the maximal value $\hat{\mu}$ of μ for which a positive solution to both (6) and (7) is possible. Note that of necessity $\hat{\mu} \leqslant \lambda$.

The conditions for the existence of quasistationary distributions, given below in Theorem 1, involve testing for the regularity or otherwise of one or other of two associated processes. These are the $\hat{\mu}$-reverse process, whose transitions rates $\mathsf{Q}^* = (q^*_{jk}, j, k \in C)$ are given by

$$q^*_{jk} = m_k q_{kj}/m_j, \qquad k \neq j, \quad j, k \in C$$
$$q^*_j \triangleq -q^*_{jj} = q_j - \hat{\mu}, \qquad j \in C$$

and the $\hat{\mu}$-dual process, which has transition rates $\bar{\mathsf{Q}} = (\bar{q}_{jk}, j, k \in C)$ given by

$$\bar{q}_{jk} = q_{jk} x_k / x_j, \qquad k \neq j, \quad j, k \in C$$
$$\bar{q}_j \triangleq -\bar{q}_{jj} = q_j - \hat{\mu}, \qquad j \in C$$

Observe that both Q^* and $\bar{\mathsf{Q}}$ are stable q-matrices over C and, owing to the $\hat{\mu}$-invariance of m and x, they are both conservative, that is,

$$\sum_{k \in C} q^*_{jk} = \sum_{k \in C} \bar{q}_{jk} = 0, \qquad j \in C$$

The $\hat{\mu}$-reverse process has a role analogous to the *time-reversed process* which arises in the theory of stationary processes.[16] The $\hat{\mu}$-dual, on the other hand, admits an interpretation as a *conditioned process*, one whose transition rates are defined conditional on the process never leaving C.[17]

The main result of the paper is the following theorem:

Theorem 1. If one of Q^* or $\bar{\mathsf{Q}}$ is regular and both of the conditions

$$\sum_{k \in C} m_k \alpha_k < \infty \tag{12}$$

and

$$\sum_{k \in C} m_k x_k < \infty \tag{13}$$

are satisfied, then the limits (4) and (5) exist and define proper probability distributions over C; the first is given by

$$m_j \alpha_j \Big/ \sum_{k \in C} m_k \alpha_k, \qquad j \in C \tag{14}$$

and the second by

$$m_j x_j \Big/ \sum_{k \in C} m_k x_k, \qquad j \in C \tag{15}$$

Before proceeding with a proof of the theorem, I shall make a number of remarks relating to it.

The condition that $\sum_k m_k x_k$ converges is necessary for (15) to define a proper probability distribution over C. It shall be seen from the proof that its major role is to establish that C possesses the property of λ-positive recurrence.[18] If this were known in advance, then one could establish that (12) and (13) are sufficient conditions for the existence of the quasistationary distributions (4) and (5) by referring to the results of Vere-Jones[19] and Flaspohler.[20] Note also that the property of λ-recurrence[18] is not used here as a premise in arriving at the conclusion that C is λ-positive recurrent, as it is, for example, in Kingman.[18] One need only check that just one of Q^* or $\bar{\mathsf{Q}}$ is regular. This condition might seem rather unusual at first sight. However, if condition (13) is satisfied, the ensuing λ-recurrence of C ensures that the regularity of one implies the regularity of the other, a fact which can easily be deduced from Theorem 2 of Pollett.[15]

I have noted that $\hat{\mu} \leqslant \lambda$, the implication being that for μ in the range $\hat{\mu} < \mu \leqslant \lambda$ there exist μ-subinvariant quantities that are not strictly μ-invariant. However, it can be seen from the proof of the theorem that if condition (13) is satisfied, the ensuing λ-recurrence of C also implies that $\hat{\mu} = \lambda$. Thus, I have provided a means of determining the decay parameter of C, at least under certain conditions, directly from Q.

Theorem 1 bears some resemblance to Corollary 2 of Flaspohler.[20] However, there the premise is that $\{q_j, j \in C\}$ be bounded. This condition is rather strong, although clearly not as stringent as the condition that C be finite. It is not satisfied, for example, by the Markov process used in modeling the autocatalytic reaction schemes described above. The condition immediately implies that Q is regular and, since $q_j^* = \bar{q}_j = q_j - \mu \leqslant q_j$, it also implies that both Q^* and $\bar{Q}$ are regular.

Corollary 2 of Pollett[15] provides sufficient conditions for the regularity of Q^* and $\bar{Q}$ in the case when Q is *regular* and so they are not appropriate for use in calculating quasistationary distributions for explosive processes. A sufficient condition for Q^* to be regular is that $\sum_k m_k$ converges, while a sufficient condition for the regularity of $\bar{Q}$ is that $\{x_j\}$ be bounded. Thus, if Q is regular and $\sum_k m_k < \infty$, then provided $\sum_k m_k x_k < \infty$, for example, if $\{x_j\}$ is bounded, then the quasistationary distributions given by (14) and (15) exist.

Proof. First observe that, by the Markov property,

$$P\{B \mid X(t) = j, X(0) = i, A_t\} = P\{B \mid X(0) = j\} = \alpha_j$$

and, using (3), that

$$P\{X(t) = j \mid X(0) = i, A_t\} = p_{ij}(t) \Big/ \sum_{k \in C} p_{jk}(t)$$

These two statements combine to give

$$P\{X(t) = j \mid X(0) = i, A_t, B\} = p_{ij}(t)\alpha_j \Big/ \sum_{k \in C} p_{ik}(t)\alpha_k \tag{16}$$

Using a similar argument, it is easy to show also that

$$P\{X(t) = j \mid X(0) = i, A_{t+s}, B\} = p_{ij}(t) \sum_{k \in C} p_{ik}(t)\alpha_k \Big/ \sum_{k \in C} p_{ik}(t+s)\alpha_k \tag{17}$$

Now if one of Q* or $\bar{Q}$ is regular, then, by Theorem 5.2 of Pollett,[17] condition (13) implies that C is λ-positive recurrent. Using Corollary 5.1 of the same paper, it follows that $\hat{\mu} = \lambda$ and so m and x are the unique λ-invariant measure and vector on C for Q. Combining Proposition 2 of Tweedie[21] and Theorem 4 of Kingman,[18] we have that

$$e^{\lambda t} p_{ij}(t) \to x_i m_j \Big/ \sum_{k \in C} m_k x_k, \qquad i, j \in C$$

Thus, multiplying the denominator and the numerator of (16) by $e^{\lambda t}$ and those of (17) by $e^{\lambda(s+t)}$ and taking the limits specified by (4) and (5), as in the proof of Theorems 1 and 2 of Flaspohler,[20] achieves the desired result.

REFERENCES

1. M. Malek-Mansour and G. Nicolis, *J. Stat. Phys.* **13**:197–217 (1975).
2. R. Gortz and D. F. Walls, *Z. Physik B* **25**:423–427 (1976).
3. D. T. Gillespie, *J. Phys. Chem.* **81**:2340–2361 (1977).
4. J. Keizer, *J. Chem. Phys.* **67**:1473–1476 (1977).
5. J. W. Turner and M. Malek-Mansour, *Physica* **93A**:517–525 (1978).
6. R. W. Parsons and P. K. Pollett, *J. Stat. Phys.* **46**:249–254 (1987).
7. G. Nicolis, *J. Stat. Phys.* **6**:195–222 (1972).
8. I. Oppenheim, K. E. Shuler, and G. H. Weiss, *Physica* **88A**:191–214 (1977).
9. S. Dambrine and M. Moreau, *Physica* **106A**:559–573 (1981).
10. S. Dambrine and M. Moreau, *Physica* **106A**:574–588 (1981).
11. N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).
12. G. E. H. Reuter, *Acta Math.* **97**:1–46 (1957).
13. J. N. Darroch and E. Seneta, *J. Appl. Prob.* **4**:192–196 (1967).
14. P. K. Pollett, Quasistationary distributions and the Kolmogorov criterion, Research report, Murdoch University (1986).
15. P. K. Pollett, *Stochastic Process. Appl.* **22**:203–221 (1986).
16. F. P. Kelly, *Reversibility and Stochastic Networks* (Wiley, London, 1979).
17. P. K. Pollett, *Adv. Appl. Prob.* **20** (1988), to appear.
18. J. F. C. Kingman, *Proc. Lond. Math. Soc. (3)* **13**:337–358 (1963).
19. D. Vere-Jones, *Aust. J. Stat.* **11**:67–78 (1969).
20. D. C. Flaspohler, *Ann. Inst. Stat. Math.* **26**:351–356 (1974).
21. R. L. Tweedie, *Q. J. Math. Oxford (2)* **25**:485–495 (1974).
22. B. Gaveau and L. S. Schulman, *J. Phys. A* **20**:2865–2873 (1987).
23. J. Greensite and M. B. Halperin, *Nucl. Phys. B* **242**:167–188 (1984).
24. R. J. McCraw and L. S. Schulman, *J. Stat. Phys.* **18**:293–301 (1978).