Quasistationary Distributions for Autocatalytic Reactions

R. W. Parsons[1] and P. K. Pollett[2]

We provide simple conditions for the existence of quasistationary distributions that can be used to describe the long-term behaviour of *open* autocatalytic reaction systems. We illustrate with reference to a particular example that the quasistationary distribution is close to the usual stationary diffusion approximation.

1. INTRODUCTION

We shall consider a stochastic model for autocatalytic reaction systems that possess two time-independent steady states, one stable and the other, corresponding to the exhaustion of a particular species, unstable. Two common examples considered previously are[1-5]

$$A + X \xrightarrow{k_1} 2X$$
$$2X \xrightarrow{k_2} B \tag{1}$$

and[6-9]

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

[1] Clinical Epidemiology Unit, Queen Elizabeth II Medical Centre, Nedlands, Western Australia, 6009.

[2] School of Mathematical and Physical Sciences, Murdoch University, Murdoch, Western Australia 6150.

each system being open with respect to both A and B. We shall suppose
that the number of molecules of species X can be adequately described by a
Markov process $(X(t), t \geqslant 0)$ whose state space consists of an absorbing
state 0 and an irreducible transient class $C = \{1, 2, 3,...\}$. Unless, excep-
tionally, $X(t)$ becomes unboundedly large, eventual absorption is certain
and ultimately all the probability is concentrated at the absorbing state.
However, this state is (macroscopically) unstable. The explanation of this
apparent anomaly lies in the fact that there are evidently two time scales in
operation. First, after a relatively short time, the system relaxes to the
stable state, and then, after a very much longer period, it eventually
evanesces.[7,10]

Several authors[7 9] have used the notion of a *quasistationary dis-
tribution* to describe the fluctuations about the stable steady state, but they
limit themselves to a finite-state birth and death (B & D) process for-
mulation that is only appropriate for dealing with closed systems in which
the number of X molecules can change by at most 1 during a reaction. In
this paper we extend their results to denumerably infinite state processes
that involve jump sizes greater than 1. In addition, we show that the
quasistationary distribution is close to the stationary diffusion
approximation of Kurtz[11,12] and Barbour.[13]

2. QUASISTATIONARY DISTRIBUTIONS

For simplicity let us suppose that we are dealing with a system in
which the number of species X cannot grow unboundedly. Under this
assumption the two most common quasistationary distributions used to
describe the long-term behavior of $(X(t), t \geqslant 0)$ are the *stationary con-
ditional quasistationary distribution*

$$\lim_{t \to \infty} P\{X(t) = j \mid X(0) = i, X(t) \neq 0\}, \qquad i, j \in C \qquad (3)$$

and the *doubly limiting conditional quasistationary distribution*

$$\lim_{t \to \infty} \lim_{s \to \infty} P\{X(t) = j \mid X(0) = i, X(s+t) \neq 0\}, \qquad i, j \in C \qquad (4)$$

Each describes the limiting probability that the process is in state j given
that (i) absorption has not occurred or (ii) will not occur in the distant
future. Under certain conditions[15,16] the limits (3) and (4) each define a
proper probability distribution $\Pi = (\pi_j, j \in C)$ that does not depend on the
starting state i. However, these conditions are at least partly expressed in
terms of the transition probabilities, which are seldom available. If C is

finite, then the quasistationary distributions can be determined by considering the eigenvector equations

$$\sum_{j \in C} u_j q_{jk} = -\mu u_k, \qquad \sum_{j \in C} q_{kj} v_j = -\mu v_k, \qquad k \in C \qquad (5)$$

where $\mathbf{Q} = (q_{jk}, j, k \geqslant 0)$ is the q-matrix of transition rates and $\mu \geqslant 0$; in accordance with convention the diagonal element q_{jj} is set to $-q_j$, where $q_j = \sum_{k \neq j} q_{jk}$ is the rate out of state j. It is always possible to find positive solutions $\mathbf{u} = (u_j, j \in C)$ and $\mathbf{v} = (v_j, j \in C)$ corresponding to the eigenvalue $-\lambda$ with maximal real part, and further, both quasistationary distributions exist[14]; the first is given by

$$\pi_j = u_j \Big/ \sum_{k \in C} u_k, \qquad j \in C \qquad (6)$$

and the second by

$$\pi_j = u_j v_j \Big/ \sum_{k \in C} u_k v_k, \qquad j \in C \qquad (7)$$

If on the other hand C is infinite, as is the case when the reaction system in question is open, the situation is far more complicated. First there are no longer finitely many eigenvalues. Rather, they usually comprise a continuum and positive eigensolutions can be obtained for at best a finite range $[0, \lambda]$ of values of μ.[16] Indeed, it may be that there are no positive eigensolutions whatsoever. The infinite case has been dealt with recently by Pollett.[17] In particular, sufficient conditions are obtained for the existence of quasistationary distributions and in the present context they amount to the following: if positive eigensolutions exist for some $\mu \geqslant 0$, and $\mathbf{u}$ and $\mathbf{v}$ are those solutions corresponding to the maximal value of μ, then the condition that both $\sum_k u_k$ and $\sum_k u_k v_k$ converge is sufficient to ensure that limits (3) and (4) exist and are given by (6) and (7). We note that the convergence of $\sum_k u_k v_k$ is necessary for (7) to be a proper probability distribution over C. However, even if it is not satisfied, it is still possible for the stationary conditional quasistationary distribution to exist.[18] In this case the conditions for existence are less straightforward. One must check that the μ-reverse q-matrix $\mathbf{Q}' = (q'_{jk}, j, k \in C)$, defined over C by $q'_{jk} = u_k(q_{kj} + \mu \delta_{jk})/u_j$, is nonexplosive (for details see Pollett[17]).

To illustrate our results, we calculated quasistationary distributions for various parameter values in each of the two reaction systems described. For brevity we shall deal here only with (1); for further illustration we refer the reader to Parsons.[21] It is clear that the only possible transitions for the process are upward jumps of size 1 and downward jumps of size 2. If

we assume that the reaction takes place in a container of unit volume, the transition rates are $q_{j,j+1} = ajk_1$, where a is the number of molecules present of species A, and $q_{j,j-2} = \frac{1}{2}j(j-1)k_2$. The eigensolutions to (5) were calculated using NAG[19] software by taking successively larger northwest-corner truncations of the q-matrix restricted to C, until the difference in the eigensolutions was adequately small (following Seneta,[20] Section 7.3). For the values $a = 1000$, $k_1 = 4$, and $k_2 = 100$ we found that the maximal value λ for μ was very close to zero. We also found that almost all of the entries in the right eigenvector were identical (from the ninth onward they were identical to six significant figures; the first eight elements were all lower than this common value by an amount of no more than 1.5%). As a result, the two types of quasistationary distribution were
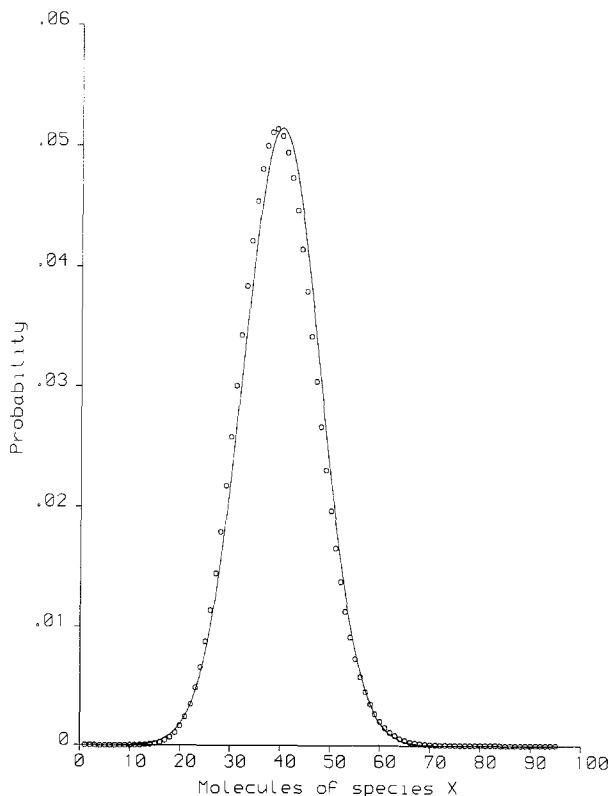

Fig. 1. Stationary conditional quasistationary distribution for example 1, with the parameter values as given in the text. (○) The exact distribution; (—) the normal approximation. The mean and variance of the exact distribution are 39.5 and 60.3, respectively, while the corresponding values for the approximate distribution are 40 and 60, respectively.

almost identical, with the difference being the greatest (although still negligible for practical purposes) in the first few elements, where the doubly limiting conditional distribution assigns slightly lower probability. The distribution evaluated using the current parameter values is illustrated in Fig. 1.

The deterministic model for this example is defined by the differential equation

$$dx/dt = F(x) = axk_1 - x^2 k_2$$

The stable deterministic steady state is the positive root x_{st} of the equation $F(x_{st}) = 0$, that is, $x_{st} = k_1 a/k_2$, which, for the current parameter values, equals 40. Notice that, as expected, the mode of the distribution is very close to this value.

On referring to the experience of other researchers (see, for example, Dunstan and Reynolds[22]) it should be no surprise that the quasistationary distributions appear to be approximately normal. Indeed, it can be shown that the process itself can be accurately approximated (in Law) by an Ornstein–Uhlenbeck (OU) process. Barbour[13] presents results that show how closely and for how long we can expect this approximation to be good for the special case of univariate and bivariate processes. The parameters of the appropriate approximating OU process can be calculated using the work of Kurtz. It is easy to show (for details see Parsons[21]) that the infinitesimal variance of the process is given by

$$\sigma_\infty^2 = -G(x_{st})/2H(x_{st})$$

where $G(x) = k_1 ax + 2k_2 x^2$ and $H(x) = k_1 a - 2k_2 x$. On substitution we find that $\sigma_\infty^2 = 3x_{st}/2$, which is in close agreement with the exact quasistationary distribution for this example and with the simulation results of Gillespie.[3] The OU approximation for the current parameter values is also shown in Fig. 1. It appears that the two distributions are very close indeed.

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. G. Nicolis, *J. Stat. Phys.* **6**:195–222 (1972).
7. I. Oppenheim, K. E. Shuler, and G. H. Weiss, *Physica* **88A**:191–214 (1977).
8. S. Dambrine and M. Moreau, *Physica* **106A**:559–573 (1981).

9. S. Dambrine and M. Moreau, *Physica* **106A**:574–588 (1981).
10. N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).
11. T. G. Kurtz, *J. Appl. Prob.* **7**:49–58 (1970).
12. T. G. Kurtz, *J. Appl. Prob.* **8**:344–356 (1971).
13. A. D. Barbour, *Adv. Appl. Prob.* **8**:296–314 (1976).
14. J. N. Darroch and E. Seneta, *J. Appl. Prob.* **4**:192–196 (1967).
15. D. C. Flashpohler, *Ann. Inst. Stat. Math.* **26**:351–356 (1974).
16. D. Vere-Jones, *Aust. J. Stat.* **11**:67–78 (1969).
17. P. K. Pollett, Reversibility, invariance and μ-invariance, Research report, Murdoch University (1986).
18. E. Seneta, *Aust. J. Stat.* **8**:92–98 (1966).
19. NAG, *FORTRAN Library Manual, Mark 11* (Numerical Algorithms Group, Oxford, 1984).
20. E. Seneta, *Non-negative Matrices and Markov Chains*, 2nd ed. (Springer-Verlag, New York, 1981).
21. R. W. Parsons, Mathematical models of chemical reactions, Ph.D. thesis, University of Wales (1985).
22. F. D. J. Dunstan and J. F. Reynolds, *J. Appl. Prob.* **18**:263–267 (1981).