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POISSONIAN STATIONARY DISTRIBUTION: A DEGENERATE CASE OF STOCHASTIC KINETICS

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There is practically no chemical reaction with independent reaction rates having Poissonian stationary (equilibrium) distribution. There exists, hovewer, a manifold of reactions with dependent reaction rates and with Poissonian stationary distribution. In this case the explicit form of the interdependence between the reaction rates is also given.

На практике не существуют химические реакции с независимыми скоростями, имеющими пуассоновское стационарное (равновесное) распределение. Однако существует совокупность реакций, скорости которых имеют пуассоновское распределение и являются взаимно зависимыми. Для этого случая дается также явная форма взаимной зависимости скоростей реакций.

INTRODUCTION

Some interest has arisen in determining the form of the equilibrium distribution in stochastic kinetics. Prigogine's surprise (/3/, p. 782) suggests the reason for his conjecture that the stationary distributions in stochastic reaction kinetics are usually Poissonian. Prigogine was able to construct a reaction with non-Poissonian stationary distribution. This need not be surprising. At first, it is easy to prove, using the results of Bartlett /1/ and Whittle /4/ that, loosely speaking, simple birth and death processe have a Poissonian stationary distrubution (PSD) if and only if their transition rates are linear (Érdi and Tóth /2/).

On the other hand, it is easy to prove (as we shall do below) for the one-dimensional case that

(i) there is no reaction with independent reaction rate constants having a PSD (with a trivial exception, see below);

(ii) there does exist a manifold of reactions of each order having a PSD.

These statements will be proven by giving the explicit relations between the reaction rate constants.

POLYNOMIAL JUMP PROCESSES WITH PSD

Let k and l be nonnegative integers, $\psi_o, \ldots, \psi_k$; $\mu_o, \ldots, \mu_l$ nonnegative real numbers; and let us define for all nonnegative integers n polinomials ψ and μ as follows:

$$\psi(n) := \sum_{i=o}^{k} \psi_i n^i, \quad \mu(n) := \sum_{i=o}^{l} \mu_i n^i \quad (\psi_k \neq 0), \ \mu_l \neq 0 \tag{1}$$

Let us consider the (one-dimensional) birth and death process with birth and death rate functions ψ and μ, respectively. Which of these processes has a PSD? A necessary and sufficient condition for this is that there exists a positive real number for which

$$P_n \ \psi(n) = P_{n+1} \mu(n+1) \ (n = 0, 1 \ldots) \tag{2}$$

holds, where

$$P_n := \lambda^n e^{-\lambda} / n!; \ n = 0, 1, \ldots \tag{3}$$

After inserting eq. (3) into (2), we obtain

$$(n + 1) \ \psi \ (n) = \lambda \mu \ (n + 1) \tag{4}$$

and this gives the necessary condition

$$l = k + 1$$

Let us insert eq. (1) into (4) and use eq. (5). Then a comparison of the coefficients of the polynomials on the two sides gives:

$$\psi_o = \lambda(\mu_o + \mu_1 + \dots + \mu_{k+1}) \tag{0'}$$

$$\psi_o + \psi_1 = \lambda(\binom{1}{o}\mu_1 + \binom{2}{1}\mu_2 + \dots + \binom{k+1}{k}\mu_{k+1}) \tag{1'}$$

$$\psi_{j-1} + \psi_j = \lambda(\binom{j}{o}\mu_j + \binom{j+1}{1}\mu_{j+1} + \dots + \binom{k+1}{k+1-j}\mu_{k+1} \tag{j'}$$

$$\psi_{k-1} + \psi_k = \lambda(\binom{k}{o}\mu_k + \binom{k+1}{1}\mu_{k+1} \tag{k'}$$

$$\psi_k = \lambda\mu_{k+1} \tag{(k+1)'}$$

Now we can say that we have an implicit system of k+2 equations for the following 2k+4 variables: λ; $\mu_{k+1}, \dots, \mu_o$; $\psi_k, \dots, \psi_o$. Let us consider as unknown the following: λ, and, if $k > 0$, $\psi_{k-1}, \psi_{k-2}, \dots \psi_o$. λ can be expressed, from eq. ((k+1)'), as

$$\lambda = \psi_k / \mu_{k+1}$$

It is clear that the remaining system of equations has a (unique, positive) solution in the ψ's. Using eqs. (k'), ..., (2') (1'), we get by induction

$$\psi_r = (\psi_k / \mu_{k+1}) \cdot \sum_{i=r+1}^{k+1} \binom{i-1}{r} \mu_i \qquad (r=0, 1, \dots, k-1) \tag{6}$$

Inserting the expressions for λ and ψ_o, into eq. (0'), $\mu_o = 0$ is obtained.

Therefore, we can relate the birth and death rates /1/ with the following reaction (which is not the only way to relate them, cf. Kurtz-type or combinatorial kinetics, and the inverse problem of reaction kinetics):

$$A \underset{\mu_1}{\overset{\psi_0}{\rightleftharpoons}} X \underset{\mu_2}{\overset{\psi_1}{\rightleftharpoons}} 2X \rightleftharpoons \ldots \rightleftharpoons kX \underset{\mu_{k+1}}{\overset{\psi_k}{\rightleftharpoons}} (k+1)\,X \tag{7}$$

(Here A is an external, constant component, and $\mu_o = 0$ is already used.)

We conclude that reaction (7) results in a PSD if and only if the respective reaction rates are interdependent and the dependence is as expressed in eq. /6/.

There is no theoretical obstacle listing the equations corresponding to (0'), (1'), ..., ((k+1)') for the six polynomials μ_1, μ_2, ψ_1, ψ_2, ϕ_{12}, ϕ_{21} in the two-dimensional case. The calculations in the two-dimensional case are the more tedious that the analogue of eq. (2), i.e. a kind of "stochastic detailed balance", does not hold.

EXAMPLES

If $k = 0$, we have $\mu_o = 0$, $\lambda = \psi_o / \mu_1$ that is $\psi(n) = \psi_o$, $\mu(n) = \mu_1 n$ and the reaction

$$A \underset{\mu_1}{\overset{\psi_o}{\rightleftharpoons}} X \tag{8}$$

Strictly speaking, this is the exceptional case where PSD results without an interdependence between the reaction rate constants.

If $k = 1$, we have $\mu_o = 0$, $\lambda = \psi_1 / \psi_2$; $\psi_o = \psi_1(\mu_1 + \mu_2)/\mu_2$ and the reaction is

$$A \underset{\mu_1}{\overset{\psi_1(\mu_1+\mu_2)/\mu_2}{\rightleftharpoons}} X \underset{\mu_2}{\overset{\psi_1}{\rightleftharpoons}} 2X \tag{9}$$

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