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Stochastic Processes

B. A. Sevast'yanov; Uspekhi Matematicheskikh Nauk, Volume VI, No 6 (46), pages 47-99. Moscow/Leningrad: Nov-Dec 1951.

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INTRODUCTION TO THE THEORY OF BRANCHING STOCHASTIC PROCESSES

B. A. Sevast'yanov

[Note: The following article represents the first section, entitled Introduction, to the report, "Theory of Branching Stochastic Processes", which appeared in the journal Uspekhi Matematicheskikh Nauk, Volume VI, No 6 (46) Nov/Dec 1951, pages 47-99. The expression "stochastic processes" is in Russian "sluchaynyye protsessy" (случайные процессы).]

In physics and chemistry occur many phenomena which are connected with the transformation of particles of one type into particles of some other types. In the study of such phenomena differential equations serve as the ordinary apparatus for their investigation. In this case the computations are carried out with respect to the mean values of the number of particles. Thus, for example, in chemistry the law of mass action permits us to derive the differential equations for the concentration of the substances taking part in the reaction.

Let us illustrate the above-mentioned by means of the following example. The photochemical reaction of the formation of HCl from the mixture of H_2 and Cl_2 proceeds according to the following scheme:

$$Cl_2 + h\nu = Cl + Cl$$
$$Cl + H_2 = H + HCl$$
$$H + Cl_2 = Cl + HCl$$
$$Cl + H_2 = H + HCl$$
$$\cdots\cdots\cdots\cdots$$

Under the action of a quantum of light the molecule Cl_2 breaks up into two atoms of chlorine, each of which starts a chain of transformations. Since rupture of the chain, thus ending the reaction of the H or Cl atoms with the mixture or the recombination of the atoms on the walls of the reaction vessel, is very unlikely, such chains will ordinarily be very long. It has been established that one quantum of light absorbed by a mixture of H_2 and Cl_2 will cause 10^5 HCl molecules to form. This fact permits us for the sake of simplicity during calculations of the very

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beginning of the reaction to consider that chain will not break. Thus, one Cl atom starts the following chain of reactions

$$Cl + H_2 = H + HCl \qquad (1)$$
$$H + Cl_2 = Cl + HCl$$
$$\cdots\cdots$$

During calculations of the initial stage of the reaction we can consider the concentrations of H_2 and Cl_2 as invariable. Taken into consideration in calculations are only those particles which are scarce at the beginning of the reaction. In our example this will be Cl and H atoms and HCl molecules, which we shall call respectively particles of types T_1, T_2 and T_3. Thus, omitting H_2 and Cl_2 we can describe reaction (1) in the following manner:

$$T_1 \rightarrow T_2 + T_3 \qquad (2)$$
$$T_2 \rightarrow T_1 + T_3 .$$

For the sake of simplicity we shall assume that both reactions proceed with the same velocity. Then for the mean values of the number of particles of types T_1, T_2 and T_3 the following system of differential equations holds:

$$\frac{dM_1}{dt} = -kM_1 + kM_2$$
$$\frac{dM_2}{dt} = -kM_2 + kM_1 \qquad (3)$$
$$\frac{dM_3}{dt} = k(M_1 + M_2) .$$

Since we are studying the chain reaction beginning with one particle of type T_1, then for $t = 0$ we have

$$M_1 = 1 \quad \text{and} \quad M_2 = M_3 = 0 . \qquad (4)$$

Solution of the system (3) for the initial conditions (4) has the form:

$$M_1 = \frac{1}{2}(1 + e^{-2kt}), \quad M_2 = \frac{1}{2}(1 - e^{-2kt}), \quad M_3 = kt .$$

Calculations carried out with respect to only the mean values of the number of particles are often insufficient. Therefore the following problem arises: to find a law of distribution of the number of particles at each moment of time of the process. Many chain processes, it turns out, can be placed under the scheme of so-called <u>branching stochastic processes</u>. This scheme often affords an effectiv

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solution of the problem. As an example we shall give a theoretic-probable picture of the process of reaction (2). Let one particle of type T_1 be transformed during an interval of time Δt with probability $p\Delta t + o(\Delta t)$ into $T_2 + T_3$, and let one particle of type T_2 be transformed during time Δt and with the same probability into $T_1 + T_3$, but let the particles of type T_3 be invariable. The state of our system will be defined by the quantity of particles of types T_1, T_2, and T_3. Designating the quantity of type T_1 by α_1 we can characterize the state of the system by the three-dimensional vector $\alpha = (\alpha_1, \alpha_2, \alpha_3)$. It is easy to see that the process being studied is a Markoff stochastic process. Let $P^{\alpha}(t)$ be the probability that at moment of time t there are α_1 particles of type T_1. The probability $P^{\alpha}(t)$ satisfies the system of differential equations

$$\frac{dP^{\alpha}}{dt} = \sum_{\beta} P^{\beta} q^{\alpha}_{\beta} \quad , \tag{5}$$

where q^{α}_{β} for $\beta \neq \alpha$ is the probability density of the transition from the state β to the state α, and q^{α}_{α} is the probability density of the escape of the system from the state α. It is easily seen that in our case q^{α}_{β} is determined by the following equations:

$$q^{(\alpha_1,\alpha_2,\alpha_3)}_{(\beta_1,\beta_2,\beta_3)} = \begin{cases} (\alpha_1+1)p & \text{if } \beta_1 = \alpha_1+1,\ \beta_2 = \alpha_2-1,\ \beta_3 = \alpha_3-1 \\ (\alpha_2+1)p & \text{if } \beta_1 = \alpha_1-1,\ \beta_2 = \alpha_2+1,\ \beta_3 = \alpha_3-1 \\ -(\alpha_1+\alpha_2)p & \text{if } \beta_i = \alpha_i \quad i = 1,2,3; \\ 0 & \text{in all remaining cases} \end{cases} \tag{6}$$

Thus, the system of equations (5) is written down in the following form:

$$\frac{dP^{\alpha}}{dt} = P^{(\alpha_1+1,\alpha_2-1,\alpha_3-1)}(\alpha_1+1)p + P^{(\alpha_1-1,\alpha_2+1,\alpha_3-1)}(\alpha_2+1)p - (\alpha_1+\alpha_2)pP^{\alpha}. \tag{7}$$

Multiplying both sides of equation (7) by $x_1^{\alpha_1}x_2^{\alpha_2}x_3^{\alpha_3}$ and summing the result obtained with respect to all possible vectors $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, we can write down an infinite system of equations (7) with the aid of the generating function

$$F(t;x_1,x_2,x_3) = \sum_{\alpha} P^{\alpha}(t)\, x_1^{\alpha_1}x_2^{\alpha_2}x_3^{\alpha_3}$$

in the form of one equation with partial derivatives of the first order

$$\frac{\partial F}{\partial t} = p(x_2x_3 - x_1)\frac{\partial F}{\partial x_1} + p(x_1x_3 - x_2)\frac{\partial F}{\partial x_2} \quad . \tag{8}$$

The solution of equation (8) must be satisfied by the following conditions:

$$F(0;x_1,x_2,x_3) = x_1 \ , \qquad F(t;1,1,1) = 1. \tag{9}$$

This equation can be solved without difficulty. We deduce at once the finite closed form of the generating function

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$$F(t;x_1,x_2,x_3) = x_1 e^{-pt}\frac{e^{px_3t}+e^{-px_3t}}{2} + x_2 e^{-pt}\frac{e^{px_3t}-e^{-px_3t}}{2}. \qquad (10)$$

Expanding (10) in powers of x_1, x_2, x_3 we find the desired probabilities:

$$p^{(1,0,2k)} = (pt)^{2k}/e^{pt}(2k)!\,, \quad p^{(0,1,2k+1)} = (pt)^{2k+1}/e^{pt}(2k+1)!\,.$$

Since we have

$$M_1(t) = \partial F(t;1,1,1)/\partial x_1\,,$$

then differentiating (8) with respect to x_1 and setting $x_1=x_2=x_3=1$ we obtain the first equation for the mathematical expectations of system (3). The remaining two equations of system (3) are obtained if we differentiate (8) with respect to x_2 and x_3 respectively. We note here that the coefficient k in system (3) is obtained equal to p.

In equation (8) the expression $px_2x_3-px_1$ serves as the coefficient of $\partial F/\partial x_1$. Here the transformation $T_1 \to T_2 + T_3$ occurs in the studied system during the time Δt with the probability $p\Delta t + o(\Delta t)$. Hence it is easy to note as a rule the composition of the coefficients of the derivatives $\partial F/\partial x_1$ and $\partial F/\partial x_2$ in the equation (8). This as a rule possesses a general character. We shall employ this significance in order to complicate to a certain extent the problem.

Closer to the real behavior of the reaction will be the assumption of the possibility of rupture of the chain. Let us assume that in the time Δt a particle of type T_1 "dies out" with the probability $q\Delta t + o(\Delta t)$ (that is, falls out of the chain reaction by joining, for example, with the mixture). Let us assume the same also for the particle of type T_2. Then in analogy with (8) we can write down for the generating function $F(t;x_1,x_2,x_3)$ the partial derivative equation

$$\frac{\partial F}{\partial t} = [px_2x_3+q-(p+q)x_1]\frac{\partial F}{\partial x_1} + [px_1x_3+q-(p+q)x_2]\frac{\partial F}{\partial x_2}, \qquad (11)$$

whose solution must satisfy the conditions (9). Differentiating (11) with respect to x_1, x_2, x_3 and setting $x_1=x_2=x_3=1$, we obtain a system of differential equations for M_1, M_2, M_3:

$$\begin{aligned} dM_1/dt &= -(p+q)M_1+pM_2 \\ dM_2/dt &= pM_1-(p+q)M_2 \\ dM_3/dt &= p(M_1+M_2) \end{aligned} \qquad (12)$$

which must be solved for initial conditions (4). The solution of (12) assumes the form $M_1 = \frac{1}{2}e^{-qt}(1+e^{-2pt})$, $M_2 = \frac{1}{2}e^{-qt}(1-e^{-2pt})$, $M_3 = \frac{p}{q}(1-e^{-qt})$.

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In particular, $M_3(\infty) = p/q$. Solving equation (11) we find the generating function $F(t; x_1, x_2, x_3)$:

$$F(t; x_1, x_2, x_3) = \frac{x_1}{2} e^{-(p+q)t}\left(e^{px_1 t} + e^{-px_1 t}\right) + \frac{x_2}{2} e^{-(p+q)t}\left(e^{px_2 t} - e^{-px_2 t}\right) + \frac{q\left[1 - e^{-(p+q)t} e^{px_3 t}\right]}{p+q-px_3} \quad (13)$$

It is easy to see that as $t \to \infty$ the particles of types T_1 and T_2 sooner or later will die out and only particles of the type T_3 will remain, the number of which will never diminish after this. From (13) it is easy to deduce that the probabilities W_m that the final number of particles of type T_3 will equal a given number m are expressed by the formula

$$W_m = \frac{q}{p+q}\left(\frac{p}{p+q}\right)^m,$$

which naturally agrees with the expression for the mathematical expectation just mentioned:

$$M_3(\infty) = p/q = \sum_{m=1}^{m=\infty} m \frac{q}{p+q}\left(\frac{p}{p+q}\right)^m.$$

Branching stochastic processes first defined in all their generality in articles by A. N. Kolmogorov and N. A. Dmitriyev (Doklady Akademii Nauk SSSR, 56, No. 1 (1947), pages 7-10), represent a theoretic-probabilistic scheme of numerous processes similar to the one just discussed. The theory of branching processes possesses an extensive literature in both this country and abroad.

In actual physical and chemical processes the premises of the theory of branching processes are disrupted because of the following reasons: a) interactions between the particles subjected to calculation (which the theory disregards), b) dependences of the chances of the particles upon their position in space (for example, during discontinuity of the chains at the walls of the vessel in the case of chemical reactions), c) dependences of the particles upon their energy (for example, in shower processes in cosmic ray studies).

However, acquaintance with the apparatus for investigating branching processes in their pure form can be of certain interest to physicists and chemists. For example, most problems considered in N. Arley's book (On the Theory of Stochastic Processes and Their Application to the Theory of Cosmic Radiations, New York: 1943, which was reprinted in the USA after its appearance in Denmark, are solved automatically without any difficulty by the application of more general methods.

END

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