Письма в ЭЧАЯ. 2008. Т. 5, № 3(145). С. 345–352

КОМПЬЮТЕРНЫЕ ТЕХНОЛОГИИ В ФИЗИКЕ

NONLINEAR FLUCTUATION-INDUCED RATE EQUATIONS FOR LINEAR BIRTH–DEATH PROCESSES

J. Honkonen

Department of Military Technology, National Defence College, Helsinki

The Fock-space approach to the solution of master equations for the one-step Markov processes is reconsidered. It is shown that in birth–death processes with an absorbing state at the bottom of the occupation-number spectrum and occupation-number independent annihilation probability occupation-number fluctuations give rise to rate equations drastically different from the polynomial form typical of birth–death processes. The fluctuation-induced rate equations with the characteristic exponential terms are derived for Mikhailov's ecological model and Lanchester's model of modern warfare.

Пересмотрено приближение пространства Фока для решения основных уравнений одношаговых марковских процессов. Показано, что в процессах рождения–уничтожения с состоянием поглощения в нижней части спектра чисел заполнения и с не зависящей от чисел заполнения вероятностью аннигиляции флуктуации чисел заполнения дают в скоростные уравнения вклад, существенно отличающийся от случая полиномиальной формы, типичной для процессов рождения–уничтожения. Получены флуктуационно-индуцированные скоростные уравнения с характерными экспоненциальными членами для экологической модели Михайлова и модели войны Ланкастера.

PACS: 02.50.Ga; 89.65.Cd

INTRODUCTION

Temporal evolution of quantities such as population density in ecology, concentration of reactants in physical chemistry and force levels in combat models in operations research are often described in terms of deterministic differential equations (rate equations). This implies the deliberate departure from the stochastic nature of the process described to arrive at simple equations. Usually, the model underlying the particular system of differential equations allows for construction of master equations for the probability density functions (PDF) of the fluctuating quantities as well. However, it often happens that it is not the full solution of these equations, which is of practical interest, but only a few moments of the random quantities, let alone those cases, when the PDF's cannot be found in a closed form. In most models the rate equations may, e.g., be inferred from the stochastic model as the equations governing the evolution of expectation values of the fluctuating quantities, when all correlations are neglected.

To illustrate this procedure, let us take as an example the classic Verhulst (or logistic) model with the rate equation

$$\frac{dn}{dt} = -\beta n + \lambda n - \gamma n^2, \tag{1}$$

in which β is the death rate of the «particles» with the population size n; λ is the birth rate and γ is the damping coefficient. The usual form of the generic master equation for the probability density functions $P(t,n)$ (with integer n) of the stochastic logistic model is

$$\frac{dP(t,n)}{dt} = \beta(n+1)P(t,n+1) + \lambda\left[(n-1) - \frac{(n-1)^2}{N}\right]P(t,n-1) - \\ - \left(\beta n + \lambda n - \frac{\lambda}{N}n^2\right)P(t,n), \quad (2)$$

where N is the «natural» size of the population. This set of equations allows the following «transport» interpretation: particles jump from states with higher occupation number $(n+1)$ to states with lower occupation number (n) with transition rates $\beta(n+1)$, and vice versa with the transition rates $\lambda n - \gamma n^2$.

Usually Eq. (2) is amended by the condition that the state with vanishing occupation number is an absorbing state and the state with the occupation number N is a reflecting state. When correlations are neglected, the stochastic logistic model (2) reproduces the rate Eq. (1) as the evolution equation for the expectation value of the occupation number. If the nonlinear term is absent in the rate Eq. (1), then it is an exact equation for the expectation value. This is because the transition rates in the model vanish together with the occupation number of the originating state. Indeed, consider the following linear birth–death model:

$$\frac{dP(t,n)}{dt} = [\alpha + \beta(n+1)]P(t,n+1) + [\kappa + \lambda(n-1)]\,P(t,n-1) - \\ - (\alpha + \beta n + \kappa + \lambda n)\,P(t,n), \quad (3)$$

with the empty state as an absorbing state. The rate equation for the expectation value $\langle n\rangle$ following from (3) is

$$\frac{d\langle n\rangle}{dt} = \kappa + (\lambda - \beta)\langle n\rangle - \alpha\,[1 - P(t,0)]\,.$$

Thus, the complete linear expression for the birth rate gives rise to terms of anticipated form, whereas the constant term in the linear death rate produces a term which does not fit in the approximation of discarding correlations. In order to obtain a closed equation for the expectation value $\langle n\rangle$, the probability of the absorbing state $P(t,0)$ should be expressed in terms of $\langle n\rangle$, which is not simple.

The aim of this paper is, first, to demonstrate that this is not an academic problem only, but there are important stochastic models sharing this feature. Second, it will be shown how a closed approximate equation for the expectation value of the occupation number may be constructed in this situation.

1. STOCHASTIC MODELS WITH DEATH RATES INDEPENDENT OF OCCUPATION NUMBER

It is a quite common feature of stochastic models in biology and chemistry that the transition rates are proportional to the occupation number of the originating state, perhaps multiplied by some polynomial in the occupation number. However, birth rates which remain finite at vanishing occupation number of the originating state do occur, but as we have seen in example (3), this does not lead to complications in the construction of rate equations from master equations.

On the contrary, models with death rates possessing an independent of the occupation number term are rare. An example is the ecological model of the Lotka–Volterra type proposed by A. S. Mikhailov [1], whose rate equations are

$$\frac{dN}{dt} = (BM - A)N, \qquad \frac{dn}{dt} = (bM - a)n, \qquad \frac{dM}{dt} = Q - GM - CN - cn. \tag{4}$$

Here, N and n are population densities of two species competing for the same type of food with the density M. Note that on the right-hand side of the third (linear) equation in (4) for the rate of change of the food density M there are both a growth term independent of all variable densities and decay terms independent of the food density M.

Another example is Lanchester's model of modern warfare, a classic model in combat modeling in operations research, in which only death rates independent of the occupation number of the originating state are present. Lanchester's models of warfare are designed to describe dynamics of gross or average combat loss rates (attrition rates). They were proposed by F. W. Lanchester in 1914 [2] and — presumably independently — by M. Osipov in 1915 [3]. A fairly detailed account and comprehensive review of various generalizations and ramifications in operations research may be found in [4]. It should also be noted that recently Lanchester's models of warfare have attracted considerable attention in ecology as well [5].

Lanchester's model of modern warfare is based on the idea of concentration of aimed friendly fire on particular enemy units at a time. This means that the enemy loss rate is independent of the enemy force level — a quantity describing the effectiveness of the army in combat — but proportional to the friendly force level. Therefore, the deterministic differential equations for the force levels of the Red Army n_r and the Blue Army n_b in Lanchester's model for modern warfare are

$$\frac{dn_r}{dt} = -\alpha_r n_b, \qquad \frac{dn_b}{dt} = -\alpha_b n_r, \tag{5}$$

where α_r and α_b are the attrition coefficients. In kinetics described by (5) there is a conservation law, the famous Lanchester's *square law*:

$$\alpha_r n_b^2 - \alpha_b n_r^2 = \text{const.} \tag{6}$$

The following discussion will be carried out for Lanchester's model of modern warfare. The corresponding results for Mikhailov's ecological model are readily inferred from those of Lanchester's model.

The generic master equations for the stochastic model of modern warfare may be constructed in the same way as those for the Verhulst model (1) with the result (see, e.g., [4]):

$$\begin{aligned}\frac{dP(t, n_r, n_b)}{dt} = \alpha_r n_b \left[P(t, n_r + 1, n_b) - P(t, n_r, n_b)\right] + \\ + \alpha_b n_r \left[P(t, n_r, n_b + 1) - P(t, n_r, n_b)\right],\end{aligned} \tag{7}$$

where n_r and n_b are the (integer) force levels of the Red and the Blue, respectively. The states in which either n_r or n_b vanishes are absorbing states.

If the initial condition is a fixed-number force level for both sides, then (7) is a finite set of coupled linear ordinary differential equations, but in indefinite number. For more challenging initial conditions like an initial Poisson distribution of force levels we arrive at an infinite set of coupled equations. This suggests that a Fock space spanned by creation and annihilation operators familiar from quantum mechanics might be useful to construct solutions without apparent dependence on the force levels (occupation numbers).

2. SOLUTION OF MASTER EQUATIONS IN FOCK SPACE

Solution of coupled master equations was first cast in a quantum-field-theoretic form by Doi [6] with subsequent reinventions by Zel'dovich and Ovchinnikov [7] and Grassberger and Scheunert [8]. For simplicity of notation, we will describe the solution of coupled master equations with the use of annihilation and creation operators in a Fock space in the example of the single-species death process with master equations obtained from (3) by putting $\kappa = \lambda = 0$.

Define the Fock space through the usual annihilation and creation operators $\hat{a}$, $\hat{a}^+$ and the basis vectors $|\, n\,\rangle$

$$\hat{a}|\,0\,\rangle = 0, \quad \hat{a}^+|\,n\,\rangle = |\,n+1\,\rangle, \quad [\,\hat{a}, \hat{a}^+] = \hat{a}\hat{a}^+ - \hat{a}^+\hat{a} = I, \tag{8}$$

with the normalization $\langle\, n\,|\,m\,\rangle = n!\delta_{nm}$. Introduce then the state vector

$$|\,\Phi\,\rangle = \sum_{n=0}^{\infty} P(t,n)|\,n\,\rangle, \qquad P(t,n) = \frac{1}{n!}\,\langle\, n\,|\,\Phi\,\rangle \tag{9}$$

for a collective description of all PDF's. From (3) and (9) the kinetic equation in the form

$$\frac{d|\,\Phi\,\rangle}{dt} = (\alpha+\beta)P(t,1)|\,0\,\rangle + \sum_{n=1}^{\infty}\{[\alpha+\beta(n+1)]P(t,n+1) - (\alpha+\beta n)P(t,n)\}\,|\,n\,\rangle \tag{10}$$

follows. The aim here is to rewrite all terms on the right-hand side in a form in which the PDF with a given occupation number n is multiplied by a basis vector with the same n without any other n dependence, e.g., $nP(t,n)|\,n\,\rangle = \hat{a}^+\hat{a}P(t,n)|\,n\,\rangle$ and $(n+1)P(t,n+1)|\,n\,\rangle = \hat{a}P(t,n+1)|\,n+1\,\rangle$ due to the definitions in (8).

For the terms in the death rate independent of n a special annihilation operator $\hat{A}$ is needed, however, with the properties $\hat{A}|\,0\,\rangle = 0$ and $\hat{A}|\,n\,\rangle = |\,n-1\,\rangle$, $n \geqslant 1$ (cf. $\hat{a}|\,n\,\rangle = n|\,n-1\,\rangle$). Note that no such complication arises for constant terms in the birth rate. The expression of this operator in terms of the usual operators $\hat{a}^+$ $\hat{a}$ is not obvious, but it may be readily checked that in the normal form the special operator is represented by the (formal) sum [9]

$$\hat{A} = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n!}\,(\hat{a}^+)^{n-1}\hat{a}^n, \tag{11}$$

which is the root of the nonlinearity brought about by this term in the rate equation for the expectation value $\langle n\rangle$.

The kinetic equation (10) may then be cast in the following operator form with the formal operator solution

$$\frac{d|\,\Phi\,\rangle}{dt} = \hat{L}(\hat{a}^+,\,\hat{a})|\,\Phi\,\rangle, \qquad |\,\Phi(t)\,\rangle = \mathrm{e}^{t\hat{L}(\hat{a}^+,\,\hat{a})}|\,\Phi(0)\,\rangle,$$

where the Liouville operator independent of the occupation number

$$\hat{L}(\hat{a}^+,\hat{a}) = (I - \hat{a}^+)(\alpha\hat{A} + \beta\hat{a})$$

has been introduced. Here, I is the identity operator.

To calculate averages of occupation-number-dependent quantities the projection vector

$$\langle\,P\,| = \sum_{n=0}^{\infty}\frac{1}{n!}\langle\,n\,| = \sum_{n=0}^{\infty}\frac{1}{n!}\langle\,0\,|\hat{a}^n = \langle\,0\,|\,\mathrm{e}^{\hat{a}} \tag{12}$$

is needed to yield

$$\langle Q(n)\rangle = \sum_{n=0}^{\infty} Q(n)P(t,n) = \langle\,P\,|Q(\hat{a}^+\hat{a})|\,\Phi\,\rangle. \tag{13}$$

It is convenient to pull the coherent-state exponential of the projection vector (12) to the right in the expectation value (13) with the aid of the relation $\mathrm{e}^{\hat{a}}\hat{a}^+ = (\hat{a}^+ + I)\,\mathrm{e}^{\hat{a}}$. Thus,

$$\langle Q(n)\rangle = \langle\,0\,|Q[(\hat{a}^+ + I)\hat{a}]\,\mathrm{e}^{t\hat{L}'(\hat{a}^+,\,\hat{a})}|\,\Phi'(0)\,\rangle, \tag{14}$$

with the shifted Liouville operator $\hat{L}'(\hat{a}^+,\,\hat{a}) = \hat{L}(\hat{a}^+ + I,\hat{a})$ and the initial-state vector $|\,\Phi'(0)\,\rangle = \sum_{n=0}^{\infty} P(0,n)(\hat{a}^+ + I)^n|\,0\,\rangle = \Phi_{\mathrm{in}}(a^+)|\,0\,\rangle$.

3. VARIATIONAL PROBLEM FOR THE GENERATING FUNCTION

To construct a perturbative expansion of the expectation value (14) decompose the Liouville operator to a free-field and an interaction part: $\hat{L}' = \hat{L}'_0 + \hat{L}'_I$, introduce time-dependent operators with free-field dynamics: $\hat{a}^{\pm}(t) = \mathrm{e}^{-t\hat{L}'_0}\hat{a}^{\pm}\,\mathrm{e}^{t\hat{L}'_0}$ to arrive at the T-exponential of the interaction picture (see, e.g., [10] for details):

$$\langle Q(n)\rangle = \langle\,0\,|Q_N[I,\hat{a}(t)]\,T\,\exp\left(\int_0^{\infty} d\tau\,L'_I(\hat{a}^+,\hat{a})\right)|\,\Phi'(0)\,\rangle,$$

where $Q_N[\hat{a}^+(t) + I, \hat{a}(t)]$ is the normal form of $Q[(\hat{a}^+ + I)\hat{a}]$. Hori's formula gives rise to the following functional form of Wick's theorem for the time-ordered exponential:

$$\langle Q(n)\rangle = \exp\left(\frac{\delta}{\delta a}\,\Delta\,\frac{\delta}{\delta a^+}\right)\left\{Q_N[1,a(t)]\,\exp\left(\int_0^{\infty} d\tau\,L'_I(a^+,a)\right)\Phi_{\mathrm{in}}(a^+)\right\}\Bigg|_{a^{\pm}\to 0},$$

with the propagator

$$\Delta(t,t') = \theta(t-t')[\hat{a}(t)\hat{a}^+(t') - \hat{a}^+(t')\hat{a}(t)].$$

Consider a slightly more general quantity, the *generating functional*

$$\begin{aligned} G(J,J^+,J_{\rm in}) &= \exp\left(\frac{\delta}{\delta a}\,\Delta\,\frac{\delta}{\delta a^+}\right)\times \\ &\times\left.\left\{\exp\left(\int\limits_0^\infty d\tau\left[\,L_I'(a^+,a) + Ja + J^+a^+\right] + J_{\rm in}\Phi_{\rm in}(a^+)\right)\right\}\right|_{a^\pm\to 0}, \end{aligned} \tag{15}$$

where J, J^+ and $J_{\rm in}$ are sources. The sources J and J^+ are functions of time, while $J_{\rm in}$ and the term $\Phi_{\rm in}(a^+)$ are time-independent. The expectation value $\langle n\rangle$ may be expressed in terms of perturbative expansions of the derivatives

$$a(t) = \frac{\delta \ln G(J^+,J,J_{\rm in})}{\delta J(t)}, \qquad a^+(t) = \frac{\delta \ln G(J^+,J,J_{\rm in})}{\delta J^+(t)}. \tag{16}$$

To infer differential equations for $a(t)$ and $a^+(t)$, it is convenient to use the generating functional of one-irreducible correlation functions defined as the (functional) Legendre transform

$$\Gamma(a^+,a,J_{\rm in}) = \ln G(J^+,J,J_{\rm in}) - a^+J^+ - aJ. \tag{17}$$

In the definition of the functional (17) it is implied that all the functions J and J^+ on the right-hand side are expressed as functionals of a and a^+ from the solution of Eq. (16). The standard rules for the construction diagrammatic expansion for the functional Γ on the basis of the representation (15) of the functional G may be found, e.g., in [10].

From the definition (17) it follows that

$$J(t) = -\frac{\delta\Gamma(a^+,a,J_{\rm in})}{\delta a(t)}, \qquad J^+(t) = -\frac{\delta\Gamma(a^+,a,J_{\rm in})}{\delta a^+(t)}.$$

These equations are the stationarity equations of the variational functional $\mathcal{F}(a^+,a,J_{\rm in})$

$$\mathcal{F}(a^+,a,J_{\rm in}) = \Gamma(a^+,a,J_{\rm in}) + a^+J^+ + aJ,$$

where J and J^+ are considered fixed parameters. At the stationarity point the functional $\mathcal{F}(a^+,a,J_{\rm in})$, obviously, coincides with the generating functional $\ln G(J^+,J,J_{\rm in})$. The point of introducing the variational functional $\mathcal{F}$ is that the dependence on the variables a and a^+ is explicit, contrary to relations in (16). Therefore, solution of the variational problem for the functional $\mathcal{F}$ allows one to obtain differential equations for a and a^+ directly. This approach also allows one to find nonperturbative solutions.

Then, instead of calculating expectation values like $\langle\hat{a}(t)\rangle$ and $\langle\hat{a}^+(t)\rangle$ perturbatively they may also be found as solutions of the stationarity equations of the functional $\mathcal{F}$, whose fluctuation-independent part is

$$\mathcal{F}(a^+,a,J_{\rm in}) = S(a^+,a) + a^+J^+ + aJ + J_{\rm in}\Phi_{\rm in}[a^+(0)] + \ldots,$$

where the ellipsis stands for terms of the Taylor expansion of $\mathcal{F}$ in $a(t)$, $a^+(t)$ and $J_{\rm in}$, whose graphical expression contains loops of propagators expressing all fluctuation effects, and S is the dynamic action:

$$S(a^+,a) = -\int\limits_0^\infty dt \int\limits_0^\infty dt'\, a^+(t) K(t,t') a(t') + \int\limits_0^\infty dt\, L_I'(a^+,a).$$

Here, K is the kernel of the differential operator of $\hat{L}_0'$: $K\Delta = 1$.

4. FLUCTUATION-IMPROVED RATE EQUATIONS FOR LANCHESTER'S MODEL OF MODERN WARFARE AND MIKHAILOV'S ECOLOGICAL MODEL

The dynamic action for Lanchester's model of modern warfare constructed according to the procedure outlined above is

$$\begin{aligned} S(a_r^+, a_r, a_b^+, a_b) = &-a_r^+\partial_t a_r - a_b^+\partial_t a_b - \\ &- \alpha_r(1+a_b^+)a_b a_r^+ \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!}(1+a_r^+)^n a_r^{n+1} - \\ &- \alpha_b(1+a_r^+)a_r a_b^+ \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!}(1+a_b^+)^n a_b^{n+1}. \end{aligned} \quad (18)$$

The contribution of the initial condition function looks especially simple in the case of Poisson-distributed initial force levels with the averages $n_{\rm r0}$, $n_{\rm b0}$. In this case the variational functional is of the form

$$\begin{aligned} &\mathcal{F}(a_r^+, a_r, a_b^+, a_b) = \\ &\quad = S(a_r^+, a_r, a_b^+, a_b) + a_r^+ J_r^+ + a_r J_r + a_b^+ J_b^+ + a_b J_b + a_r^+(0) n_{\rm r0} + a_b^+(0) n_{\rm b0} + \ldots \end{aligned}$$

The stationarity equations for the action (18) have a solution with $a_r^+ = a_b^+ = 0$, in which case $a_r = \langle n_r \rangle$ and $a_b = \langle n_b \rangle$ and obey the following pair of equations:

$$\frac{da_r}{dt} = -\alpha_r a_b (1 - \mathrm{e}^{-a_r}), \qquad \frac{da_b}{dt} = -\alpha_b a_r (1 - \mathrm{e}^{-a_b}). \quad (19)$$

For large average force levels the exponentials are negligible in Eq. (19) and deterministic Lanchester's equations (5) for force levels are recovered. For generic values of force levels these exponentials approximate the contribution of the PDF of the absorbing states to the rate equation.

From (19) a conservation law follows in the form:

$$\begin{aligned} &\alpha_r \left[a_b^2 + 2a_b \ln\left(1 - \mathrm{e}^{-a_b}\right) - 2\mathrm{Li}_2\left(\mathrm{e}^{-a_b}\right)\right] - \\ &\qquad - \alpha_b \left[a_r^2 + 2a_r \ln\left(1 - \mathrm{e}^{-a_r}\right) - 2\mathrm{Li}_2\left(\mathrm{e}^{-a_r}\right)\right] = \text{const}, \end{aligned}$$

which replaces Lanchester's square law (6). Here, Li_2 is the dilogarithm.

Relations in (19) also provide a quantitative statement that the fluctuation-induced deviations from deterministic Lanchester's equations are exponentially small in the average force levels. Inspection of the structure of the perturbation expansion reveals that the exponential fall-off survives to higher orders of perturbation theory. A similar effect is produced by fluctuations also in Mikhailov's model, whose rate equations in (4) are replaced by

$$\frac{dN}{dt} = (BM-A)N, \quad \frac{dn}{dt} = (bM-a)n, \quad \frac{dM}{dt} = Q-GM-CN\left(1-\mathrm{e}^{-M}\right)-cn\left(1-\mathrm{e}^{-M}\right)$$

with a significant effect for small values of the food density M.

CONCLUSION

A variational approach within the Fock-space method of solution of master equations has been used to find rate equations for averages of fluctuating occupation numbers in birth–death processes. It has been shown that in the case of a death rate independent of the occupation number a special nonpolynomial annihilation operator (11) is needed within the Fock-space approach. Nonpolynomial nonlinearities in the dynamic action of the Fock-space method are shown to appear due to this, even if the transition rates are linear functions of the occupation numbers. These nonlinearities show in the rate equations as well, which should be taken into account, when the underlying stochastic process is described at the level of rate equations. Fluctuation-improved rate equations have been proposed for both Lanchester's model of modern warfare and Mikhailov's ecological model.

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