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Orthogonal Polynomial Solutions of the Fokker–Planck Equation

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We have tabulated the form of the coefficients $g_1(x)$ and $g_2(x)$ as well as the boundary values $[a, b]$ of the Fokker–Planck equation

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}[g_1(x)P(x,t)] + \frac{\partial^2}{\partial x^2}[g_2(x)P(x,t)], \qquad a \leqslant x \leqslant b$$

for which the solution can be written as an eigenfunction expansion in the classical orthogonal polynomials. We also discuss the problem of finding solutions in terms of the discrete classical polynomials for the differential difference equations of stochastic processes.

KEY WORDS: Fokker–Planck equation; stochastic processes; orthogonal polynomials.

1. INTRODUCTION

The starting point of many investigations of time-dependent phenomena in the statistical description of physical processes is the master equation[1]

$$\partial P(x, t \mid x_0)/\partial t = \int A(x, x')P(x', t \mid x_0)\, dx' \tag{1}$$

Here $P(x, t \mid x_0)$ is the conditional probability that the system which started in state x_0 at time zero evolves to state x at time t, and $A(x, x')$ is the

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transition rate from x' to x. Often this nonlocal integral equation is approximated by a local differential equation. If the transition rate is expanded in a Kramers–Moyal series[2] about $x = x'$ and one truncates at the second term, the Fokker–Planck (FP) equation is obtained[1]

$$\frac{\partial P(x, t \mid x_0)}{\partial t} = \frac{\partial^2}{\partial x^2} [g_2(x)P(x, t \mid x_0)] - \frac{\partial}{\partial x} [g_1(x)P(x, t \mid x_0)] \quad (2)$$

with

$$g_1(x) = \int (x - x')\, A(x, x')\, dx', \qquad g_2(x) = \int (x - x')^2\, A(x, x')\, dx' \quad (3)$$

The purpose of this paper is to classify the solutions of this equation with appropriate boundary conditions which can be related to the classical orthogonal polynomials. That is, we wish to find the coefficients $g_2(x)$ and $g_1(x)$ which permit one to express the solution of Eq. (2) as an eigenfunction expansion in these polynomials. We place two physical restrictions on the system: First, only systems that conserve probability are considered, and second, we require that a nonzero equilibrium solution exist.

Several examples of the Fokker–Planck equation (2) are known which have solutions in terms of classical orthogonal polynomials. Thus, the Ornstein-Uhlenbeck process on an infinite line has an eigenfunction expansion in terms of Hermite polynomials.[3] The vibrational relaxation of harmonic oscillators in the continuous (high temperature) limit leads to an expansion in terms of Laguerre polynomials.[4] The energy relaxation of a hard-sphere Rayleigh gas (Brownian motion) also has a solution in terms of a Laguerre polynomial expansion.[5] A number of other examples can be found in the literature.[1,3]

We felt it would be useful to find and tabulate the values of $g_1(x)$ and $g_2(x)$ and the appropriate boundary conditions which yield all the members of the set of FP equations with orthogonal polynomial solutions. Hopefully, this will eliminate much unproductive labor in the future by other workers in hunting for what might be nonexisting polynomial solutions of FP equations.

2. FOKKER–PLANCK EQUATIONS

In this section we consider the forward Kolmogorov equation[1] for the conditional probability $P(x, t \mid x_0)$

$$\frac{\partial^2}{\partial x^2} [g_2(x)P(x, t \mid x_0)] - \frac{\partial}{\partial x} [g_1(x)P(x, t \mid x_0)] = \frac{\partial P(x, t \mid x_0)}{\partial_t}, \quad a \leqslant x \leqslant b \quad (4)$$

For the initial condition on $P(x, t \mid x_0)$ we take

$$P(x, 0 \mid x_0) = \delta(x - x_0) \quad (5)$$

To conserve probability in the space $a \leqslant x \leqslant b$, we use the boundary condition

$$[(\partial/\partial x)g_2(x)P(x, t \mid x_0) - g_1(x)P(x, t \mid x_0)]_{x=a,b} = 0 \tag{6}$$

which corresponds to zero flux at the boundaries. The probability is normalized to unity:

$$\int_a^b P(x, t \mid x_0)\, dx = 1 \tag{7}$$

The normalized equilibrium solution of Eq. (4) with the boundary conditions of Eq. (6) is

$$\begin{aligned} P_e(x) \equiv P(x, \infty \mid x_0) = &\left(\exp - \int^x \frac{g_2'(y) - g_1(y)}{g_2(y)}\, dy\right) \\ &\times \left\{\int_a^b \left[\exp - \int^x \frac{g_2'(y) - g_1(y)}{g_2(y)}\, dy\right] dx\right\}^{-1} \end{aligned} \tag{8}$$

where the primes indicate derivatives with respect to the argument.

In more compact form Eq. (4) can be rewritten as

$$\mathscr{L}P = \partial P/\partial t \tag{9}$$

where

$$\mathscr{L}P \equiv \frac{\partial}{\partial x}\left[P_e(x)g_2(x)\frac{\partial}{\partial x}\frac{P(x, t \mid x_0)}{P_e(x)}\right] \tag{10}$$

The differential operator $\mathscr{L}$ with the boundary conditions of Eq. (6) is not self-adjoint. We define

$$G(x, t \mid x_0) \equiv P_e^{-1/2}(x)P(x, t \mid x_0) \tag{11}$$

Then G satisfies

$$\bar{\mathscr{L}}G = \partial G/\partial t \tag{12}$$

where

$$\bar{\mathscr{L}} \equiv g_2(x)\frac{d^2}{dx^2} + g_2'(x)\frac{d}{dx} + \frac{1}{2}\left\{g_2''(x) - g_1'(x) - \frac{[g_2'(x) - g_1(x)]^2}{2g_2(x)}\right\} \tag{13}$$

and $\bar{\mathscr{L}}$ with the boundary conditions (6) is self-adjoint. The solution of Eq. (12) can therefore be expressed as an eigenfunction expansion in terms of the eigenfunctions $G_n(x)$ and eigenvalues λ_n of $\bar{\mathscr{L}}$. Thus

$$G(x, t \mid x_0) = \sum_n c_n(x_0)\, G_n(x)e^{\lambda_n t} \tag{14}$$

where

$$\bar{\mathscr{L}}G_n = \lambda_n G_n \tag{15}$$

The G_n must satisfy the boundary conditions (6). Since the differential operator $\mathscr{L}$ together with the boundary conditions is self-adjoint, the G_n form a complete orthogonal set:

$$\int_a^b G_n(x)\, G_m(x)\, dx = h_n \delta_{nm} \tag{16}$$

Using the initial condition

$$G(x, 0 \mid x_0) = P_e^{-1/2}(x)\, \delta(x - x_0) \tag{17}$$

and Eq. (16) we can evaluate $c_n(x_0)$ to find

$$G(x, t \mid x_0) = \sum_n [G_n(x) G_n(x_0)\, P_e^{-1/2}(x_0) e^{\lambda_n t}/h_n] \tag{18}$$

We are interested in the set of FP equations for which

$$G_n(x) G_m(x) = W(x) f_n(x) f_m(x) \tag{19}$$

where $f_n(x)$ is a monic $[f_0(x) = 1]$ polynomial of degree n. The polynomials $f_n(x)$ form a complete orthogonal set with respect to the weight function $W(x)$ on the interval $[a, b]$. Since we have specified the existence of a nonzero equilibrium distribution, we must have $\lambda_0 = 0$. It then follows from Eqs. (8), (11), (18), and (19) that

$$W(x) = P_e(x) \tag{20}$$

To determine the $g_2(x)$ and $g_1(x)$ that will give rise to a particular set of polynomials, it is convenient to define

$$H(x, t \mid x_0) \equiv P_e(x) P(x, t \mid x_0) \tag{21}$$

Then from Eqs. (8) and (10)

$$\mathscr{F} H = \partial H / \partial t \tag{22}$$

where

$$\mathscr{F} \equiv g_2(x)(d^2/dx^2) + g_1(x)(d/dx) \tag{23}$$

The coefficients $g_2(x)$ and $g_1(x)$ are now chosen such that

$$\mathscr{F} f_n = \lambda_n f_n \tag{24}$$

In terms of the polynomials f_n and the eigenvalues λ_n, we then obtain

$$P(x, t \mid x_0) = \sum_n [P_e(x) f_n(x) f_n(x_0)\, e^{\lambda_n t}/h_n] \tag{25}$$

where h_n is defined by Eq. (16). In Table 1 we list the range $[a, b]$, the coefficients, eigenvalues, and equilibrium solutions for the classical orthogonal polynomials.[7] It is interesting to note that $g_1(x)$ is linear in x in all cases. This has important connotations for the physical processes described by FP equations of the type discussed here.[6]

The sum in Eq. (5) has been evaluated in closed form for only two of the polynomials. If the $f_n(x)$ are the Hermite polynomials,[8] then

$$P(x, t \mid x_0) = \frac{1}{[2\pi(1 - e^{-4t})]^{1/2}} \exp\left[-\frac{(x - x_0 e^{-2t})^2}{1 - e^{-4t}}\right] \tag{26}$$

For the generalized Laguerre polynomials[8]

$$P(x, t \mid x_0) = \left(\frac{x}{x_0}\right)^{\alpha/2} e^{-x} \frac{e^{\alpha t/2}}{1 - e^{-t}} \left(\exp - \frac{x + x_0}{e^t - 1}\right) I_\alpha\left(\frac{2(x x_0 e^{-t})^{1/2}}{1 - e^{-t}}\right) \tag{27}$$

where $I_\alpha(z)$ is the modified Bessel function.

If one encounters a Fokker–Planck equation of the form

$$\frac{\partial^2}{\partial x^2} [b_2(x)P(x, t \mid x_0)] - \frac{\partial}{\partial x} [b_1(x)P(x, t \mid x_0)] = \frac{\partial P(x, t \mid x_0)}{\partial t} \tag{28}$$

where b_2 and b_1 do not correspond to entries in Table I, a transformation of variables may bring Eq. (28) into one of the standard forms. For the most general transformation we let

$$y = \int^x dx' \, [g_2(x')/b_2(x')]^{1/2} \tag{29}$$

Then, if we define $p(y, t \mid y_0) \equiv P(x, t \mid x_0)$, we find

$$\frac{\partial^2}{\partial y^2} [g_2(y)p(y, t \mid y_0)] - \frac{\partial}{\partial y} [g_1(y)p(y, t \mid y_0)] = \frac{\partial p(y, t \mid y_0)}{\partial t} \tag{30}$$

provided that

$$\frac{1}{2} g_2'(x) \left[\frac{b_2(x)}{g_2(x)}\right]^{1/2} + \left[2b_2'(x) - b_1(x) - \frac{1}{2}\frac{b_2'(x)}{g_2'(x)}\right] \left[\frac{g_2(x)}{b_2(x)}\right]^{1/2} = 2g_2'(y) - g_1'(y) \tag{31}$$

and

$$b_2''(x) - b_1'(x) = g_2''(y) - g_1'(y) \tag{32}$$

and where the left-hand sides of Eqs. (31) and (32) must be expressed as functions of y. It should be noted that the transformation (29) may also cause a change in the value of the boundary points a, b. This needs to be checked before the results of Table I can be applied.

Table 1. Coefficients, Eigenvalues, Range [a, b], and Equilibrium Solutions for the Classical Orthogonal Polynomials

Polynomial	a	b	$g_2(x)$	$g_1(x)$	$P_e(x)$	λ_n	h_n
$P_n^{(\alpha,\beta)}(x)$, $\alpha > -1, \beta > -1$ (Jacobi)	-1	1	$1 - x^2$	$\beta - \alpha - (\alpha+\beta+2)x$	$(1-x)^\alpha(1+x)^\beta$	$-n(n+\alpha+\beta+1)$	$\dfrac{2^{\alpha+\beta+1}}{(2n+\alpha+\beta+1)} \dfrac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{n!\Gamma(n+\alpha+\beta+1)}$
$C_n^{(\alpha)}(x)$, $\alpha > -1/2$ (Gegenbauer)	-1	1	$1 - x^2$	$-(2\alpha + 1)x$	$(1 - x^2)^{\alpha-(1/2)}$	$-n(n + 2\alpha)$	$\dfrac{\pi 2^{(1-2\alpha)}\Gamma(n + 2\alpha)}{n!(n + \alpha)[\Gamma(\alpha)]^2}, \alpha \neq 0$
$T_n(x)$ (Chebyshev, first kind)	-1	1	$1 - x^2$	$-x$	$(1 - x^2)^{-1/2}$	$-n^2$	$\pi/2, n \neq 0; \pi, n = 0$
$U_n(x)$ (Chebyshev, second kind)	-1	1	$1 - x^2$	$-3x$	$(1 - x^2)^{1/2}$	$-n(n + 2)$	$\pi/2$
$P_n(x)$ (Legendre)	-1	1	$1 - x^2$	$-2x$	1	$-n(n + 1)$	$2/(2n + 1)$
$L_n^{(\alpha)}$, $\alpha > -1$ (Generalized Laguerre)	0	∞	x	$\alpha + 1 - x$	$e^{-x}x^\alpha$	$-n$	$\Gamma(\alpha + n + 1)/n!$
$H_n(x)$ (Hermite)	$-\infty$	∞	1	$-2x$	$\exp -x^2$	$-2n$	$\sqrt{\pi}2^n n!$

3. DIFFERENTIAL DIFFERENCE EQUATIONS

The question arises whether an analogous classification scheme for classical discrete polynomials can be worked out for the differential difference equations (dde) of stochastic processes. The discrete state space analog of the FP equation (4) is

$$\frac{dP(l, t)}{dt} = a_{l,l+1}\, P(l+1, t) + a_{l,l-1}\, P(l-1, t) - (a_{l-1,l} + a_{l+1,l})P(l, t) \quad (33)$$

where $P(l+j, t)$ is the probability that the system is in state $(l+j)$ at time t and where the $a_{l,j}$ are the transition rates from state j to l. We now ask for the solutions of Eq. (33) in terms of the discrete classical polynomials $F_n(l)$, i.e.,

$$P(l, t) = \sum_n c_n F_n(l) e^{\lambda_n t} \quad (34)$$

in analogy with the eigenfunction expansion (14). A careful study of the literature[9] shows that almost all classical discrete polynomials satisfy difference equations whose coefficients $a_{l,j}$ are nonpositive over part or all of the permissible range of l values. The coefficients $a_{l,j}$ then cannot be interpreted as transition rates (which must necessarily be positive) and the differential difference equations of the form (33) with solutions (34) do not describe stochastic processes. The only exception is the Gottlieb polynomial[10] which is the solution to a differential difference equation with positive coefficients over the whole allowed range of l.[11]

By appropriate limiting processes one can transform the differential difference equation (we consider here any of the set of dde with positive coefficients) into Fokker–Planck equations of the form (2). This transformation, depending upon the form of the coefficients $a_{l,j}$, can give rise to the coefficients $g_1(x)$ and $g_2(x)$ listed in Table I. Some examples of such transformations have been worked out by Karlin and McGregor.[12] In the "diffusion approximation" some differential difference equations may thus have solutions in terms of the classical orthogonal polynomials. How well such "diffusion approximation" solutions approximate the solutions of the original differential difference equation remains an open question.

NOTE ADDED

After this paper was completed our attention was called to the fact that in 1962 Wong and Thomas covered essentially the same ground, except for our discussion of differential difference equations, in a paper published in an applied mathematics journal.[13] Upon the suggestion of a number of our "chemical and physical" colleagues working in stochastic processes we have decided to publish this paper despite the overlap with the work of Wong and Thomas, since their work apparently is not familiar to the statistical physics fraternity.

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