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FOR A STOCHASTIC NONLINEAR ADVECTION EQUATION

RONALD E. MEYERS, EDWARD E. O'BRIEN, AND L. RIDGWAY SCOTT

September 1977

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ABSTRACT

An equation for the probability density function (p.d.f.) for the solution of advection-reaction equations is derived in the limit of white noise advection. An exact solution, consisting of a lognormal distribution, is found under appropriate initial conditions. It is also shown, via an example, how to compute a general reacting p.d.f. from a known p.d.f. for the nonreacting case by discretizing a certain exponential operator.

DERIVATION OF THE PROBABILITY DENSITY FUNCTION FOR A STOCHASTIC NONLINEAR ADVECTION EQUATION

1. INTRODUCTION

In this report, we consider the solution of a stochastic advection-reaction equation. Our interest in this subject arose out of a study of models of atmospheric pollution,¹ where diffusion also plays an important role. The results derived here may be viewed as a model with the diffusion neglected, but we emphasize that, although molecular diffusion is a small effect in the atmosphere, it cannot be ignored in stochastic problems. A model including diffusion has been given by two of the authors in an earlier publication.²

Our main result consists of a limit theorem for an advection-reaction equation, in the limit of small fluctuations in the advecting vector field. The reactive problem is reduced to a nonreactive one by introducing the probability density for the stochastic solution. The corresponding limit theorem for the homogeneous advection equation is based on the results obtained by Khas'minskii³ and Papanicolaou et al.^{4,5} on stochastic ordinary differential equations (o.d.e.'s). In the case of a linear reaction, we recover the well known model of "reacting with the mean" that is used in current pollution models; however, when the reaction is nonlinear, reacting with the mean is shown to be invalid.

We make no attempt here at rigor, since our main results (Section 3) are purely formal. The third-named author plans a mathematical treatment of this subject at a later date.

2. A LIMIT THEOREM FOR THE HOMOGENEOUS ADVECTION EQUATION

Let ε be a positive parameter and consider the Cauchy problem defining $u = u^\varepsilon$ by

$$\begin{aligned} u_t + \varepsilon \mathbf{F} \cdot \nabla u &= 0; \quad t \geq 0, \quad x \in \mathbf{R}^n, \quad \omega \in \Omega; \\ u(x, 0; \omega) &= f(x); \quad x \in \mathbf{R}^n, \quad \omega \in \Omega; \end{aligned} \quad (2.1)$$

where ω labels a particular member of the ensemble of events in our probability space Ω , $\mathbf{F} = \mathbf{F}(x, t; \omega)$ is a given (random) advection velocity, and u is the resulting random process that we wish to study in the limit $\varepsilon \downarrow 0$. Since (2.1) can be solved by the method of characteristics, our problem is reduced to the study of random o.d.e.'s of the form

$$\begin{aligned} \dot{x}^\varepsilon(s; \omega, x^0, t) &= \varepsilon \mathbf{F}(x^\varepsilon(s; \omega, x^0, t), t-s; \omega), \quad 0 \leq s \leq t; \\ x^\varepsilon(0; \omega, x^0, t) &= x^0 \end{aligned} \quad (2.2)$$

[recall that $u(x^0, t; \omega) = f(x^\varepsilon(t; \omega, x^0, t))$]. Stratonovich⁶ reasoned that, under very general hypotheses on the vector field $\mathbf{F}$, x^ε tends to a diffusion process on time scales

proportional to ε^{-2} . Although the attempt by Stratonovich⁷ at a rigorous proof of this fact was incomplete, it led to a series of papers in which limit theorems are rigorously established. The first of these seems to have been by Khas'minskii³ and the most recent by Papanicolaou and Kohler⁵ (which may be checked for intermediate references). We now give a description of the principal hypotheses required by these results.

Let $\mathcal{P}$ denote the probability measure on Ω , and let $\langle \varphi \rangle$ denote the mean of a random variable φ :

$$\langle \varphi \rangle \equiv \int_{\Omega} \varphi(\omega) d\mathcal{P}(\omega). \quad (2.3)$$

We assume that coordinates (x, t) have been chosen so that $\langle \mathbf{F} \rangle \equiv 0$. It is also necessary to assume that the statistics of the vector field $\mathbf{F}$ are stationary in time because of the time shift-reversal in the definition (2.2) of x^s (i.e., because t enters as a parameter). To derive a limit theorem, we must assume a *mixing condition*: suppose there is a function $\rho(t)$ tending (sufficiently fast) to zero as $t \uparrow \infty$ such that

$$\rho(t) \geq \mathcal{P}\{\mathbf{F}(x, t) \in V\} - \mathcal{P}\{\mathbf{F}(x, t) \in V \mid \mathbf{F}(y, 0) \in W\} \quad (2.4)$$

for all $x, y \in \mathbf{R}^n$ and all (measurable) subsets V, W of $\mathbf{R}^n$, where the second term on the r.h.s. is a conditional probability. $\rho(t)$ is an estimate of the relative independence of $\mathbf{F}(t)$ from $\mathbf{F}(0)$; $\rho \downarrow 0$ "sufficiently fast" if, e.g., $\rho(t) = O(t^{-2-\delta})$ for arbitrary $\delta > 0$. Now define

$$\begin{aligned} a_{ij}(x) &= \lim_{T \uparrow \infty} \frac{1}{T} \int_0^T \int_0^\sigma \langle F_i(x, \sigma) F_j(x, s) \rangle ds d\sigma, \\ b_j(x) &= \lim_{T \uparrow \infty} \frac{1}{T} \int_0^T \int_0^\sigma \left\langle \sum_{i=1}^n F_i(x, \sigma) \frac{\partial F_i}{\partial x_j}(x, s) \right\rangle ds d\sigma. \end{aligned} \quad (2.5)$$

Define $\bar{u} = \bar{u}(x, t)$ as the solution to the deterministic problem

$$\begin{aligned} \frac{\partial \bar{u}}{\partial t} &= \varepsilon^2 \left(\sum_{i,j=1}^n a_{ij} \frac{\partial^2 \bar{u}}{\partial x_i \partial x_j} + \sum_{j=1}^n b_j \frac{\partial \bar{u}}{\partial x_j} \right); \quad x \in \mathbf{R}^n, \quad t \geq 0, \\ \bar{u}(x, 0) &= f(x), \quad x \in \mathbf{R}^n. \end{aligned} \quad (2.6)$$

Assume that the spatial derivatives (up to a certain order; 4 is sufficient) of f , $\mathbf{F}$, a_{ij} , and b_j are all bounded and have certain limiting properties as $|x| \rightarrow \infty$. Let $T > 0$ and $L > 0$. Then:

THEOREM. $\lim_{\varepsilon \downarrow 0} |\langle u \rangle - \bar{u}| = 0$, uniformly for $|x| \leq L$ and $t \in [0, T/\varepsilon^2]$.

In fact, in refs. 4 and 5 it is shown that there is a constant $C = C(f, \mathbf{F}, a_{ij}, b_j, T, L)$, such that

$$|\langle u(x, t) \rangle - \bar{u}(x, t)| \leq C\varepsilon$$

for $|x| \leq L$ and $t \in [0, T/\varepsilon^2]$. Of course, it is only for $t \sim T/\varepsilon^2$ that either u or $\bar{u}$ differs appreciably from f . Note that if $\text{div } \mathbf{F} = 0$, then

$$b_j = \sum_{i=1}^n \frac{\partial a_{ij}}{\partial x_i},$$

and the equation for $\bar{u}$ is in divergence form:

$$\bar{u}_t = \varepsilon^2 \sum_{i,j=1}^n \frac{\partial}{\partial x_i} \left(a_{ij} \frac{\partial \bar{u}}{\partial x_j} \right).$$

3. DERIVATION OF THE PROBABILITY DENSITY FUNCTION (p.d.f.) EQUATION FOR THE NONLINEAR ADVECTION EQUATION

Consider the system of initial value problems

$$\begin{aligned} u_t^i(x, t; \omega) + \mathbf{F}(x, t; \omega) \cdot \nabla u^i(x, t; \omega) &= R^i(u^1(x, t; \omega), \dots, u^m(x, t; \omega)), \\ u^i(x, 0; \omega) &= f^i(x), \end{aligned} \quad (3.1)$$

for $x \in \mathbf{R}^n$, $t \geq 0$, $\omega \in \Omega$, and $i = 1, \dots, m$, where $\mathbf{F}$ is a random vector field as in the last section and R is a deterministic function of m variables, i.e., independent of x , t , and ω . Let $\rho(x, t, v; \omega)$ be the associated *fine-grained density* given by

$$\rho(x, t, v; \omega) = \delta(u(x, t; \omega) - v), \quad (3.2)$$

where $u = (u^1, \dots, u^m)$ and $v \in \mathbf{R}^m$. For each $x \in \mathbf{R}^n$, $t \geq 0$, and $\omega \in \Omega$, $\rho(x, t; \omega)$ is a measure on v -space ($\mathbf{R}^m$). It satisfies the differential equation

$$\rho_t + \mathbf{F} \cdot \nabla_x \rho + \nabla_v \cdot (R \rho) = 0 \quad (3.3)$$

in the sense that, for any $\varphi \in C_0^\infty(\mathbf{R}^m)$,

$$\begin{aligned} \left(\frac{\partial \rho}{\partial t} + \mathbf{F} \cdot \nabla_x \rho + \nabla_v \cdot (R \rho), \varphi \right) &\equiv \frac{\partial}{\partial t} \int \varphi d\rho + \mathbf{F} \cdot \nabla_x \int \varphi d\rho - \int R \cdot \nabla_v \varphi d\rho \\ &= \frac{\partial}{\partial t} \varphi(u) + \mathbf{F} \cdot \nabla_x \varphi(u) - R(u) \cdot (\nabla_v \varphi)(u) \\ &= \nabla_v \varphi(u) \cdot [u_t + \mathbf{F} \cdot \nabla_x u - R(u)] = 0. \end{aligned} \quad (3.4)$$

The *probability density function* P for u is given by

$$P(x, t, v) = \langle \rho(x, t, v) \rangle; \quad (3.5)$$

for example, for any φ ,

$$\begin{aligned} \int \varphi(v) dP(x, t, v) &= \int \int \varphi(v) d\rho(x, t, v; \omega) d\omega, \\ &= \int \varphi(u(x, t; \omega)) d\omega = \langle \varphi(u(x, t)) \rangle. \end{aligned} \quad (3.6)$$

It is not known in general whether P is indeed a function rather than just a measure, i.e., that $\langle d\rho \rangle = P dv$, but the example in Section 5 indicates this possibility. We are unable to determine a general set of equations for P , but, by analogy with the results

in the previous section, we show that as the magnitude of the vector field $\mathbf{F}$ tends to zero, P tends to the solution $\bar{P}$ of the equations:

$$\bar{P}_t - \sum_{i,j=1}^n a_{ij} \frac{\partial \bar{P}}{\partial x_i \partial x_j} - \sum_{j=1}^n b_j \frac{\partial \bar{P}}{\partial x_j} + \nabla_v \cdot (R\bar{P}) = 0, \quad t \geq 0, \\ \bar{P}(x, 0, v) = \delta(f(x) - v), \quad x \in \mathbb{R}^n, \quad v \in \mathbb{R}^m, \quad (3.7)$$

where a_{ij} and b_j ; $i, j = 1, \dots, n$ are given by (see Section 2)

$$a_{ij}(x) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \int_0^\sigma \langle F_i(x, \sigma) F_j(x, s) \rangle ds d\sigma, \quad (3.8a)$$

and

$$b_j(x) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \int_0^\sigma \langle \nabla F_j(x, \sigma) \cdot \mathbf{F}(x, s) \rangle ds d\sigma. \quad (3.8b)$$

To see this, we introduce the fine-grained density (f.g.d.) ρ^* for the *conservative* or homogeneous advection equation. Let u^* be the solution of the equations (in vector form)

$$u_t^* + \mathbf{F} \cdot \nabla u^* = 0, \quad t \geq 0; \quad u^*(t=0) = f. \quad (3.9)$$

As before, define $\rho^*(x, t, v; \omega) = \delta(u^*(x, t, \omega) - v)$; it follows that ρ^* satisfies

$$\rho_t^* + \mathbf{F} \cdot \nabla_x \rho^* = 0, \quad t \geq 0, \quad (3.10)$$

with $\rho = \rho^*$ when $t = 0$. Define a linear operator A by

$$Ag \equiv -\nabla_v \cdot (Rg). \quad (3.11)$$

We then have $\rho = e^{tA} \rho^*$: since A is independent of x and t ,

$$\begin{aligned} \frac{\partial}{\partial t} (e^{tA} \rho^*) &= A(e^{tA} \rho^*) + e^{tA} \rho_t^* \\ &= A(e^{tA} \rho^*) + e^{tA} (-\mathbf{F} \cdot \nabla_x \rho^*) \\ &= A(e^{tA} \rho^*) - \mathbf{F} \cdot \nabla_x (e^{tA} \rho^*), \\ &= -\nabla_v \cdot (R(e^{tA} \rho^*)) - \mathbf{F} \cdot \nabla_x (e^{tA} \rho^*), \end{aligned} \quad (3.12)$$

that is, $e^{tA} \rho^*$ satisfies the same equation as ρ . Since they agree at $t=0$, we have $\rho = e^{tA} \rho^*$ for all $t \geq 0$.

Now, define $P^* = \langle \rho^* \rangle$. By analogy with the results in the previous section, we conclude that as the magnitude of the fluctuations of $\mathbf{F}$ tends to zero, P^* tends to the solution $\bar{P}^*$ of the initial value problem

$$\bar{P}^*_t - \sum_{i,j=1}^n a_{ij} \frac{\partial^2 \bar{P}^*}{\partial x_i \partial x_j} - \sum_{j=1}^n b_j \frac{\partial \bar{P}^*}{\partial x_j} = 0, \quad t \geq 0, \\ \bar{P}^*(x, 0, v) = \delta(f(x) - v), \quad x \in \mathbb{R}^n, \quad v \in \mathbb{R}^m. \quad (3.13)$$

We emphasize that the proof that $P^* \rightarrow \bar{P}^*$ is by analogy only, since a rigorous proof requires extension of the results of Section 2 to measures like ρ .

As in (3.12), it follows that $\bar{P} = e^{tA} \bar{P}^*$. Since A is deterministic,

$$P \equiv \langle \rho \rangle = e^{tA} \langle \rho^* \rangle = e^{tA} P^* . \quad (3.14)$$

Thus $P - \bar{P} = e^{tA}(P^* - \bar{P}^*)$, and the convergence $P \rightarrow \bar{P}$ follows from $P^* \rightarrow \bar{P}^*$.

Up to now, we have considered only deterministic initial data $f(x)$. Suppose f is random but statistically independent of the advection velocity F . Thus $f = f(x; \omega')$, where ω' represents an event in a probability space Ω' of events that are independent of the ensemble Ω . Let P' be the probability measure for Ω' . The probability space for the stochastic process u is now the product space $\Omega \times \Omega'$ with probability measure $P \times P'$. The probability density for u can be determined as follows:

$$\begin{aligned} P(x, t, v) &= P \times P' \{ u(x, t; \omega, \omega') = v \} , \\ &= \int \int_{\Omega \times \Omega'} \delta[u(x, t; \omega, \omega') - v] dP(\omega) dP'(\omega') , \\ &= \int_{\Omega'} P(x, t, v; \omega') dP'(\omega') , \end{aligned}$$

where $P(x, t, v; \omega')$ is the probability density for u given deterministic initial data $f(x; \omega')$. Since the limiting equation (3.7) for $P(x, t, v; \omega')$ is linear, we conclude that $P(x, t, v)$ also tends, in the limit of small F , to the solution of (3.7) with initial data given by

$$\begin{aligned} P(x, 0, v) &= P \times P' [u(x, 0; \omega, \omega') = v] , \\ &= P' [f(x; \omega') = v] , \end{aligned}$$

that is, $P(x, 0, v)$ is simply the probability density for f . To summarize, when the initial data are nondeterministic (but independent of F) with probability density $Q(x, v)$, the limiting probability density $\bar{P}(x, t, v)$ for the solution u of (3.1) satisfies

$$\begin{aligned} \bar{P}_t - a_{ij} \bar{P}_{,ij} - b_j \bar{P}_{,j} + \nabla_v \cdot (R \bar{P}) &= 0 , \quad t \geq 0 . \\ \bar{P} &= Q , \quad t = 0 . \end{aligned}$$

4. COMPARISON WITH REACTION WITH THE MEAN

One of the most popular approximations to the mean $\langle u \rangle$ of the solution of (3.1) is the solution $\bar{u}$ of the initial value problem (in vector form)

$$\begin{aligned} \bar{u}_t - \sum_{i,j=1}^n a_{ij} \frac{\partial^2 \bar{u}}{\partial x_i \partial x_j} - \sum_{j=1}^n b_j \frac{\partial \bar{u}}{\partial x_j} &= R(\bar{u}) , \quad t \geq 0 ; \\ \bar{u}(t=0) &= f , \end{aligned} \quad (4.1)$$

where (a_{ij}) and (b_j) are given by (3.8). This is obtained simply by juxtaposing the results of Section 2 with the approximation $\langle R(u) \rangle \sim R(\langle u \rangle)$. The results of the previous section allow us to compute $\langle u \rangle$, at least in the limit $F \rightarrow 0$:

$$\langle u \rangle(x, t) = \int P(x, t, v) v dv, \quad (4.2)$$

where P is given by (3.7) (we are dropping the bar over P). Multiplying (3.7) by v and integrating, we see that $\langle u \rangle$ satisfies

$$\begin{aligned} \langle u \rangle_t - \sum_{i,j=1}^n a_{ij} \frac{\partial^2 \langle u \rangle}{\partial x_i \partial x_j} - \sum_{j=1}^n b_j \frac{\partial \langle u \rangle}{\partial x_j} &= - \int v [\nabla \cdot (RP)] dv, \\ &= \int RP dv \quad \text{for } t \geq 0. \end{aligned}$$

Thus, we see that (for nonlinear R) we cannot in general expect that $\bar{u} = \langle u \rangle$, since this would imply

$$R \left(\int v P(x, t, v) dv \right) = \int R(v) P(x, t, v) dv \quad \text{for all } x, t.$$

5. AN EXAMPLE: SOLUTION OF THE P^* EQUATION

The meaning of (3.10) is that if the p.d.f. of the conservative equation is known, then the reactive p.d.f. can be determined. The next section deals with the numerical aspects of discretizing the exponential operator $\exp[t \nabla_v \cdot (R \quad)]$, but here we concentrate on one case where $\bar{P}^*$ can be determined exactly. We shall assume that $m=n=1$, $a_{11}=1$, $b_1=0$, and $f(x)=e^x$. For each $v \in \mathbf{R}$, $\bar{P}^*$ satisfies $\bar{P}_t^* - \bar{P}_{xx}^* = 0$ with $\bar{P}^*(x, 0, v) dv = \delta(f(x) - v)$; hence $\bar{P}^*(x, 0, v) dx = (dx/dv) \delta(f(x) - v)$, where $x = x(v)$ is the inverse relation to $v = f(x)$. Thus

$$\bar{P}^* = \sum_{\substack{x \in \mathbf{R} \\ f(x)=v}} G_x \frac{dx}{dv},$$

where G_x is the Green's function for the heat equation with singularity at x :

$$G_x(y, t) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{(y-x)^2}{4t}\right).$$

Note that $f(x)=v$ if and only if $x=\log v$. Therefore, $\bar{P}^*(x, t, v)=0$ for $v \leq 0$, and for $v > 0$,

$$\bar{P}^*(x, t, v) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{(x - \log v)^2}{4t}\right) \frac{1}{v};$$

that is, for each x, t , $\bar{P}^*$ is lognormal.

Generalizing this to the case $m=2$ of two conservative species with

$$f_1(x) = f_2(x) = e^x,$$

we see that $\bar{P}^*(x, t, v, w)$ is lognormal, but $\bar{P}^*(x, t, v, w) = 0$ if $v \neq w$.

6. DISCRETIZATION OF THE EXPONENTIAL OPERATOR

Let us consider a single species, second order reaction, i.e., $R(u) = ku^2$, $k \in \mathbf{R}$. Recall that A is the operator defined by

$$Ag \equiv \frac{d}{du} [ku^2 g(u)], \quad (6.1)$$

that is, A is the operation of multiplication by ku^2 followed by differentiation. Writing

$$e^{tA} = \sum_{n=0}^{\infty} \frac{(tA)^n}{n!}, \quad (6.2)$$

we see that we can approximate $e^{tA}g$ by the finite sum

$$e^{tA}g \sim \sum_{n=0}^N \frac{(tA)^n g}{n!} = \left\{ I + \frac{1}{N} tA \left[I + \frac{1}{N-1} tA(\dots) \right] \right\} g, \quad (6.3)$$

and further we can approximate d/du by a finite difference operator to obtain an efficient method for the approximate calculation of $e^{tA}g$. To see how well this method may work, we consider here the fundamental question of convergence of the approximation (6.3).

Let us assume that $g(u)$ is analytic for u in the open interval $0 < u < \infty$, which is satisfied, e.g., if g is lognormal as a function of u . We must estimate $A^n g(u)$, $u > 0$. We have

$$A^n g(u) = (ku)^n \sum_{j=0}^n \beta_j^n u^j g^{(j)}(u), \quad (6.4)$$

where β_j^n are positive integers. It is easy to see that $\beta_n^n = 1$; $\beta_0^n = 2^n$; $\beta_j^{n+1} = \beta_{j-1}^n + (n+j+2)\beta_j^n$; and hence that $\beta_j^n < 3^n n! / j!$ by induction. Therefore,

$$\frac{|A^n g(u)|}{n!} \leq |3ku|^n \sum_{j=0}^n \frac{|u^j g^{(j)}(u)|}{j!}. \quad (6.5)$$

The radius of convergence of the power series

$$\sum \frac{x^j g^{(j)}(u)}{j!}$$

is at least u , so for any $\rho < 1$, there is a finite number

$$G(\rho, u) \left[\equiv \sum_{j=0}^{\infty} \frac{(\rho u)^j |g^{(j)}(u)|}{j!} \right],$$

such that

$$\frac{|A^n g(u)|}{n!} \leq \frac{|3ku|^n}{\rho^n} G(\rho, u). \quad (6.6)$$

Thus the series $e^{tA}g(u)$ has a radius of convergence at least $\rho/3kt$; since ρ was arbitrary, we conclude that the radius is at least $1/3kt$. The factor 3 is unimportant, and

probably not optimal. What is relevant is that the radius is finite and shrinks as t and k increase.

Note that the series (6.2) diverges at $t \rightarrow \infty$. This can be remedied by a multistep procedure as follows: we write

$$e^{tA}g = \underbrace{e^{(t/\eta)A} [e^{(t/\eta)A} (\dots)]}_j g, \quad j \text{ times}$$

i.e., we first calculate $e^{(t/\eta)A}g \equiv g_1$, then $e^{(t/\eta)A}g_1 \equiv g_2$, etc., until we arrive at $g_j = e^{(t/\eta)A}g_{j-1} = e^{tA}g$.

If $g \equiv 0$ for $u < 0$, as is the case when g is lognormal, then we may use the fact that $g^{(n)}(0) = 0$ for all n in calculating (6.3). For example, if we choose to approximate d/du by the formula

$$\frac{d}{du} g(u) \sim \frac{g(u) - g(u-h)}{h},$$

then the values

$$\{A^n g(i\Delta u) : i = 1, 2, \dots, I\}$$

may be determined from

$$\{A^{n-1}g(i\Delta u) : i = 1, 2, \dots, I\}.$$

However, if centered differencing

$$\frac{d}{du} g(u) \sim \frac{g(u+h) - g(u-h)}{2h}$$

is used, only the values $\{A^n g(i\Delta u) : i \leq I-1\}$ may be determined. Thus, if we wish to calculate (3.3) at I points, we must begin with g at $I+N$ points. We shall leave to the reader the analysis of the error introduced by replacing d/du by finite difference operators.

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