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The backward Kolmogorov equation for the statistical distribution of coagulating droplets

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Abstract. The backward Kolmogorov equation is established and solved for a Markovian system of coagulating droplets. The resulting probability generating function of the total number of droplets coincides with the expression recently obtained by Williams from the forward equation. Thus the equivalence of the two approaches is verified for a system whose evolution implies a probability balance giving rise to terms nonlinear in the state variable.

It is shown that the backward equation lends itself to being solved directly in terms of moments of any order, whereas the forward equation shows in this respect the problem of closure.

1. Introduction

In a recent paper published in this journal (Williams 1979), the statistical distribution of coagulating droplets was studied, assuming that they form a discrete Markov system in continuous time. For the first time an exact solution was obtained for the time-dependent probability distribution of the total number of droplets irrespective of their volume. The fundamental equation solved in that work was constructed from a probability balance according to the scheme suggested by Bartlett (1962), and is actually the forward Kolmogorov equation (FKE) for the stochastic process considered.

It is well known that a probability balance can also be set up in a manner such as to lead to the backward Kolmogorov equation (BKE) (Feller 1968).

It is the purpose of the present paper to establish and solve the BKE for the probability distribution of droplets in suspension under the assumptions introduced by Williams to make the problem tractable. To this end, the droplets will again be considered to be uniformly mixed in space, to undergo only binary collisions, to stick together and conserve the effective size after a collision.

Although it is commonly claimed that the backward approach is entirely equivalent to the forward approach, the former seems to be less frequently used. Thus one of the motivations of this work is to confirm, in a case where an exact solution exists, that the two approaches indeed yield the same result.

The second motivation is to show, especially in a case such as the present one where the probability balance introduces terms nonlinear in the state variables due to the interaction of the droplets among themselves, that the solution of the backward equation is attained in a perhaps more direct fashion. For instance, purely matrix

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methods substitute for the resort to special functions that is required for the solution of the forward equation.

Finally, the backward equation will be shown not to suffer from the problem of closure, i.e. the inability to calculate the statistical averages of the distribution from a closed set of equations, which affects the forward equation.

2. General theory of the backward approach

We denote by $P(n, t|N, \tau)$ the conditional probability that the total number of droplets is n at time t, given that it was N at time $\tau < t$. If the droplets are assumed to form a Markovian system, this probability satisfies the Chapman–Kolmogorov equation (Feller 1968), namely

$$P(n, t|N, \tau-\Delta\tau) = \sum_{N'} P(N', \tau|N, \tau-\Delta\tau)P(n, t|N', \tau) \tag{1}$$

with the summation extended to all possible values of the total number of droplets N' at time τ between $\tau-\Delta\tau$ and t. Considering that in $\Delta\tau$ two droplets either collide or do not, the infinitesimal transition probability is

$$P(N', \tau|N, \tau-\Delta\tau) = \beta N(N-1)\,\Delta\tau\delta_{N',N-1} + [1-\beta N(N-1)\,\Delta\tau]\delta_{N'N} \tag{2}$$

where δ is the Kronecker symbol, β is the constant binary collision rate and thus $\beta N(N-1)$ represents the collision probability per unit time. Inserting equation (2) in equation (1), simplifying and letting $\Delta\tau \to 0$ yields the backward differential equation for the conditional probability,

$$\frac{\partial}{\partial\tau}P(n, t|N, \tau) = \beta N(N-1)[P(n, t|N, \tau) - P(n, t|N-1, \tau)], \tag{3}$$

with the boundary condition at the final time t

$$P(n, t|N, t) = \delta_{nN}. \tag{4}$$

Introducing the probability generating function for the total number of droplets n at time t,

$$F(x, t|N, \tau) = \sum_{n=0}^{\infty} P(n, t|N, \tau)x^n, \tag{5}$$

where x is a dummy variable, multiplying equation (3) by x^n and summing over n, one obtains the backward differential equation for the generating function,

$$\frac{\partial}{\partial\tau}F(x, t|N, \tau) = \beta N(N-1)[F(x, t|N, \tau) - F(x, t|N-1, \tau)]. \tag{6}$$

The boundary condition imposed on equation (6) stems from equations (4) and (5) and is

$$F(x, t|N, t) = x^N. \tag{7}$$

The solution of equations (6) and (7) for $N = 1$ is

$$F(x, t|1, \tau) = x, \tag{8}$$

which can also be obtained from equation (5) since on physical grounds $P(n, t|1, \tau) =$

δ_{n1}. Letting $N=2, 3, \ldots$ and recalling equation (8), equation (6) can be recast in the matrix form

$$\frac{\partial}{\partial \tau}|F\rangle = \boldsymbol{M}|F\rangle + |u\rangle, \tag{9}$$

where $|F\rangle$ is the column vector whose hth component is

$$F(x, t|h+1, \tau), \qquad h = 1, 2, \ldots, N-1, \tag{10}$$

$\boldsymbol{M}$ is the bidiagonal matrix whose elements are

$$M_{hk} = \beta h(h+1)(\delta_{hk} - \delta_{h-1,k}), \qquad h, k = 1, 2, \ldots, N-1, \tag{11}$$

and $|u\rangle$ is the $(N-1)$-row vector defined by

$$|u\rangle = \mathrm{col}(-2\beta x \quad 0 \quad 0 \quad 0 \ldots 0). \tag{12}$$

According to equation (7), the boundary condition for equation (9) is

$$\lim_{\tau \to t} |F\rangle = |g\rangle, \tag{13}$$

where $|g\rangle$ is the column vector whose hth component is

$$g_h = x^{(h+1)}, \qquad h = 1, 2, \ldots, N-1. \tag{14}$$

The general solution of equation (9) is

$$|F\rangle = \mathrm{e}^{-\boldsymbol{M}(t-\tau)}|g\rangle - \left(\int_\tau^t \mathrm{d}\tau' \, \mathrm{e}^{-\boldsymbol{M}(\tau'-\tau)}\right)|u\rangle,$$

which, setting the time origin at the initial time ($\tau = 0$), becomes

$$|F\rangle_{\tau=0} = \mathrm{e}^{-\boldsymbol{M}t}|g\rangle - \left(\int_0^t \mathrm{d}\tau' \, \mathrm{e}^{-\boldsymbol{M}\tau'}\right)|u\rangle. \tag{15}$$

To proceed further, one needs to evaluate the exponential function of the matrix $\boldsymbol{M}$ in equation (15). This will be accomplished through the spectral decomposition of the matrix $\boldsymbol{M}$.

3. Spectral decomposition of matrix $\boldsymbol{M}$

Matrix $\boldsymbol{M}$ has $N-1$ distinct eigenvalues that are its main diagonal elements M_{hh}. Hence it can be decomposed as

$$\boldsymbol{M} = \boldsymbol{SDQ}, \tag{16}$$

where $\boldsymbol{D}$ is the diagonal matrix with elements

$$D_{hk} = M_{hh}\delta_{hk}, \qquad h, k = 1, 2, \ldots, N-1, \tag{17}$$

$\mathbf{S}$ is the matrix whose columns $|S_{.i}\rangle$ are the $N-1$ eigenvectors of the matrix $\boldsymbol{M}$ and

$$\boldsymbol{Q} = \boldsymbol{S}^{-1}. \tag{18}$$

The calculation of the eigenvectors is carried out starting from their definition, namely

$$\boldsymbol{M}|S_{.i}\rangle = M_{ii}|S_{.i}\rangle, \qquad i = 1, 2, \ldots, N-1, \tag{19}$$

whence one obtains, using equation (11), the following recurrence formula for the elements of the matrix $\boldsymbol{S}$:

$$[j(j+1)-i(i+1)]S_{ji}=j(j+1)S_{j-1,i}, \qquad i,j=1,2,\ldots,N-1.$$

From this equation it is easy to show that S_{ji} vanishes for $j\leqslant i-1$ and is proportional to S_{ij} for $j\geqslant i+1$; moreover, one can choose $S_{jj}=1$ since the eigenvalues contain an arbitrary multiplicative constant according to equation (19). Thus, after some simplifications, the elements of the matrix $\boldsymbol{S}$ can be written

$$\underset{j,i=1,2,\ldots,N-1}{S_{ji}} = \begin{cases} \dfrac{j!\,(j+1)!\,(2i+1)!}{i!\,(i+1)!\,(j-i)!\,(i+j+1)!} & \text{for } j\geqslant i, \\ 0 & \text{for } j\leqslant i-1\ (i>1). \end{cases} \tag{20}$$

The inversion of the matrix $\boldsymbol{S}$ is more conveniently performed using equation (16), which can be written

$$\boldsymbol{QM}=\boldsymbol{DQ},$$

whence one obtains, using equations (11) and (17), the following recurrence formula for the elements Q_{jr} of the matrix $\boldsymbol{S}^{-1}$:

$$[r(r+1)-j(j+1)]Q_{jr}=(r+1)(r+2)Q_{j,r+1}, \qquad j,r=1,2,\ldots,N-1.$$

From this equation it is easy to show that Q_{jr} vanishes for $j\leqslant r-1$ and is proportional to Q_{jj} for $j\geqslant r+1$. On the other hand, this latter, with the help of the relation

$$\sum_{i=1}^{N-1} S_{ji}Q_{ir}=\delta_{jr} \tag{21}$$

which comes from equation (18), and using equation (20), turns out to be one. Thus after some simplifications the elements of the matrix $\boldsymbol{S}^{-1}$ can be written

$$\underset{j,r=1,2,\ldots,N-1}{Q_{jr}} = \begin{cases} \dfrac{(-1)^{j-r}j!\,(j+1)!\,(j+r)!}{r!\,(r+1)!\,(j-r)!\,(2j)!} & \text{for } j\geqslant r, \\ 0 & \text{for } j\leqslant r-1\ (r>1). \end{cases} \tag{22}$$

Equation (21) allows us also to find a relation, useful in the sequel, satisfied by the elements S_{ji} and Q_{ir} in the range of indices where neither of them vanish. In fact, using equations (20) and (22), equation (21) reduces to

$$\sum_{i=r}^{j} S_{ji}Q_{ir}=\delta_{jr} \qquad \text{for } j\geqslant r,$$

namely, after some calculations, to the identity

$$\sum_{i=r}^{j}(-1)^{i-r}\frac{(2i+1)(i+r)!}{(j-i)!\,(i+j+1)!\,(i-r)!}=\delta_{jr} \qquad \text{for } j\geqslant r. \tag{23}$$

Analogously, another useful identity is obtained from the relation

$$\sum_{i=1}^{N-1} Q_{ji}S_{ir}=\delta_{jr},$$

which also comes from equation (18). Using equations (20) and (22), after some calculations this leads to

$$\sum_{i=r}^{j} (-1)^{j-i} \frac{(j+i)!}{(j-i)!(i-r)!(i+r+1)!} = \frac{\delta_{jr}}{2r+1} \qquad \text{for } j \geq r. \tag{24}$$

4. Solution of the backward equation

The exponential function of the matrix $\boldsymbol{M}$ can be written in terms of its eigenvalues and eigenvectors as

$$\mathrm{e}^{-\boldsymbol{M}t} = \boldsymbol{S}\boldsymbol{D}'\boldsymbol{Q}, \tag{25}$$

where $\boldsymbol{D}'$ is the diagonal matrix with elements

$$D'_{hk} = \exp(-M_{hh}t)\delta_{hk}, \qquad h, k = 1, 2, \ldots, N-1. \tag{26}$$

Inserting equations (25), (26) and the analogous ones for time τ' in equation (15) and carrying out the integration, the solution of the backward matrix equation (9) becomes

$$|F\rangle_{\tau=0} = \boldsymbol{S}\boldsymbol{D}'\boldsymbol{Q}|g\rangle - \boldsymbol{S}\boldsymbol{D}''\boldsymbol{Q}|u\rangle, \tag{27}$$

where $\boldsymbol{D}''$ is the diagonal matrix with elements

$$D''_{hk} = \frac{1-\exp(-M_{hh}t)}{M_{hh}}\delta_{hk}, \qquad h, k = 1, 2, \ldots, N-1. \tag{28}$$

Now we can explicitly write the expression of the probability generating function of the total number of droplets at time t, given that there were N at time zero. In fact, the last row of equation (27) is immediately evaluated to be

$$F(x, t|N, 0) = \sum_{i=1}^{N-1} S_{N-1,i}\left(D'_{ii} \sum_{r=1}^{i} Q_{ir}x^{r+1} + 2\beta x D''_{ii}Q_{i1}\right),$$

where equations (10), (26), (14), (28) and (12) were used and contraction of the range of the second sum was possible on account of the properties of the Q_{ir}'s. After substituting for the several parameters from equations (20), (22), (26), (28) and (11), the RHS of the equation above is easily reduced to its final form through some computational steps which feature the inversion of the first two sums and a simplification based on identity (23). At last one obtains

$$F(x, t|N, 0) = N!(N-1)! \sum_{r=0}^{N-1} \frac{x^{r+1}}{r!(r+1)!} \sum_{i=r}^{N-1} (-1)^{i-r} \frac{(2i+1)(i+r)!\,\mathrm{e}^{-\beta i(i+1)t}}{(N+i)!(N-i-1)!(i-r)!}. \tag{29}$$

This equation expresses the generating function as a polynomial in the dummy variable. The coefficient of the power x^{r+1} is the conditional probability $P(r+1, t|N, 0)$, $r = 0, 1, 2, \ldots, N-1$, and coincides with that obtained by Williams (1979) solving the forward equation. The generating function of equation (29) satisfies the boundary condition (7), namely $F(x, 0|N, 0) = x^N$, and the well known property $F(x=1, t|N, 0) = 1$. We point out that, for the verification of these relations, the use of the identities (23) and (24) obtained in § 3 as a by-product of the main procedure is fundamental.

5. Backward equation and closure problem

Instead of solving the backward matrix equation (9), thus obtaining the complete probability distribution, one might solve for the moments of the distribution directly. Differential equations for the vectors of the factorial moments and corresponding boundary conditions are established after repeatedly differentiating equations (9), (13) and (14) with respect to x and setting $x = 1$.

In so doing, one obtains for the vector of the factorial moment of any order a differential equation formally equal to equation (9); its solution at the initial time $\tau = 0$ will be given by equation (27) after substituting for $|g\rangle$ and $|u\rangle$ their differentials with respect to x of appropriate order evaluated at $x = 1$.

This conclusion is to be compared with what happens when the procedure of obtaining equations for the moments is carried out on the forward equation (Williams 1979). There the problem of closure arises, namely the equation for any moment contains moments of higher order and it is impossible to obtain a closed set of equations.

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