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Introduction of the characteristic function in stochastic dynamic modelling

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ABSTRACT

The probability characteristic function is used to generalize Epstein's stochastic dynamic prediction model. The time-differencing scheme results in an infinite system of equations which is closed by a quasi-normal procedure. This system yields an explicite approximation to the common or arbitrary marginal characteristic function, which in turn may be transformed to an estimation of the density function. The results are illustrated for Lorenz's minimum hydrodynamic equations.

1. Introduction

Since Freiberger and Grenander (1965) in their fundamental work had raised the idea of stochastic generalization of the hydrodynamic equations, many studies have dealt with this topic. The chief purpose of such an extension is to pursue the propagation of uncertainties mainly caused by inaccurate initialization. The stochastic dynamic equations indeed proved rather fruitful in investigation of the predictability of certain physical systems (Epstein, 1969; Gleeson, 1970; Fleming, 1971b), the energy flows and the more realistic expression of various forcing processes (Fleming, 1971a, 1972). In these studies the stochastic dynamic equations have been usually derived by direct use of the expected value operator or by means of Gleeson's continuity equation (Gleeson, 1966), which actually originates from the principle that the total integral of the probability density function $f(t; X) = f(t; x_1, x_2, \ldots, x_N)$ over the entire N-dimensional phase space is conserved

$$\frac{\partial f(t;X)}{\partial t} + \nabla \cdot (G(X) f(t;X)) = 0 \qquad (1)$$

where vector-function $G = (G_1, G_2, \ldots, G_N)$ denotes the right-hand sides of the hydrodynamic equations transformed to a specific form

$$\dot{x}_p = \sum_{q=1}^{N} \sum_{r=1}^{N} a_{pqr} x_q x_r - \sum_{q=1}^{N} b_{pq} x_q + c_p$$
$$= G_p(X) \quad p = 1, 2, \ldots, N \qquad (2)$$

The atmospheric prognostic equations can be simplified in such a way utilizing spectral methods as shown by Lorenz (1963a).

According to Epstein (1969) the approximate stochastic dynamic equations extending (2) are obtained from (2) bearing in mind the definition of the probability moments $\mu_p = Ex_p$, $\mu_{ps} = Ex_p x_s$, etc.

$$\dot{\mu}_p = \sum_q \sum_r a_{pqr} \mu_{qr} - \sum_q b_{pq} \mu_q + c_p$$

$$\dot{\mu}_{ps} = \sum_q \sum_r a_{pqr} \mu_{qrs} - \sum_q b_{pq} \mu_{qs} + c_p \mu_s$$
$$+ \sum_q \sum_r a_{sqr} \mu_{qrp} - \sum_q b_{sq} \mu_{qp} + c_s \mu_p \qquad (3)$$

Although the time-dependent first- and second-order moments yielded a certain basis for the investigation of the predictability and other characteristics of a general spectral model in the above-mentioned articles, e.g. by evaluating of the standard deviations, both the more advantageous probability prediction mainly in the case of weakly stable systems, or in the environment of weakly stable initial conditions, and the finer measurements of the "indefiniteness" of the distribution, simply by the variance, more precisely by conditional variances, a system of confidence intervals or statistical entropy, claim a direct approximation to the density function. Only in some extra-regular cases of the probability distributions may one exclusively develop the first moments as the most probable values. Some studies concerned with the earth's climate (Lorenz, 1968; Dedenbach, 1977) suggest that models of the atmospheric phenomena have a single steady-stable solution, i.e. it seems that the real atmospheric system is actually "transitive". In spite of such a hypothesis both experimentally and numerically general-circulation models were constructed that evolved into several different stable states depending on the forcing and boundary conditions (Fultz et al., 1959; Lorenz, 1963b). Consequently under a stochastic dynamic prediction scheme an indefinite stochastically given initial state may develop into a random state with density function possessing a few local maxima. In this case the consideration of the only mean value and the variance for one fixed variable cannot reflect the real nature of the investigated phenomena and the internal instabilities of the model and the numerical approximation. To meet these requirements we propose another way for setting up the stochastic model.

2. The generalized stochastic dynamic equations

Let us consider the characteristic function of the process $X = X(t)$

$$\phi(t; Y) = E \exp\left(i \sum_{s=1}^{N} x_s y_s\right) \tag{4}$$

where $i = \sqrt{-1}$ is the complex unit, $Y = (y_1, y_2, \ldots, y_N)$. The mean square derivative of (4) with respect to time (Gihman and Skorohod, 1974) may be expressed in the form

$$\dot{\phi} = E \exp\left(i \sum_s x_s y_s\right) \sum_p i y_p x_p$$

Substituting (2) we obtain a closed stochastic dynamic equation for the characteristic function

$$\dot{\phi} = \sum_{p=1}^{N} y_p \left(-i \sum_q \sum_r a_{pqr} \phi_{qr} - \sum_q b_{pq} \phi_q + i c_p \phi\right) \tag{5}$$

where we used the notations $\phi_q = \partial\phi/\partial y_q$, $\phi_{qr} = \partial^2\phi/\partial y_q \partial y_r$. It is actually a complex form of Gleeson's continuity equation applied to (2). Now it is possible to carry out such a solution of (5) that immediately provides approximate values of some first moments of the process $X(t)$ simultaneously with an estimator for $\phi(t; X)$ characterizing the whole distribution. Following this goal the solution of eq. (5) will be calculated through a centred difference formula

$$\phi(t + \tau; Y) = \phi(t - \tau; Y) + 2\dot{\phi}(t; Y)\tau \tag{6}$$

where τ denotes the time step. Eq. (5) shows that the time derivative $\dot{\phi}(t; Y)$ may be expressed as linear function of up to 2nd-order partial derivatives of ϕ with respect to the independent variables $y_1, y_2, \ldots, y_N$. Operating by (5) the time derivatives of terms ϕ_j, ϕ_{jk} are consecutively, with repeated substitution, expressible as polynomials of up to 4th-order partial derivatives of the characteristic function ϕ. We close this approximate system with the difference equation for the 3rd-order terms

$$\begin{aligned}
\phi_j(t + \tau; Y) &= \phi_j(t - \tau; Y) + 2\dot{\phi}_j(t; Y)\tau \\
\phi_{jk}(t + \tau; Y) &= \phi_{jk}(t - \tau; Y) + 2\dot{\phi}_{jk}(t; Y)\tau \\
\phi_{jkl}(t + \tau; Y) &= \phi_{jkl}(t - \tau; Y) + 2\dot{\phi}_{jkl}(t; Y)\tau
\end{aligned} \tag{7}$$

Certainly at $t = 0$ only the uncentred formula is appropriate in (6) and (7). The new time derivatives in turn are deduced using repeatedly (5), e.g.

$$\begin{aligned}
\dot{\phi}_j = \sum_p y_p &\left(-i \sum_q \sum_r a_{pqr} \phi_{qrj} - \sum_q b_{pq} \phi_{qj} + i c_p \phi_j\right) \\
&+ \left(-i \sum_q \sum_r a_{jqr} \phi_{qr} - \sum_q b_{jq} \phi_q + i c_j \phi\right)
\end{aligned} \tag{8}$$

3. The quasi-normal closure

Now we need a closure procedure relating ϕ_{jklm} and ϕ_{jklmn} to lower-order terms. Otherwise, adopting the same method to compute the 4th- and 5th-order derivatives as in (6) and (7) would introduce higher-order terms. For this purpose we adopt Fleming's (1971a) closure type. Due to this quasi-normal technique the following relations are accepted that are actually valid for multidimensional normally distributed variables

$$\phi^3 \phi_{jklm} - \phi^2 \Omega^{(3)}_{jklm} + \phi\Omega^{(2)}_{jklm} - 3\phi_j\phi_k\phi_l\phi_m$$
$$= \phi^4[(\phi^*_{jk} - \phi^*_j\phi^*_k)(\phi^*_{lm} - \phi^*_l\phi^*_m) + (\phi^*_{jl} - \phi^*_j\phi^*_l)(\phi^*_{km} - \phi^*_k\phi^*_m) + (\phi^*_{jm} - \phi^*_j\phi^*_m)(\phi^*_{kl} - \phi^*_k\phi^*_l)] \quad (9)$$

where the star (*) denotes the value of the marked function at $Y = \mathbf{0}$, i.e. $y_1 = 0, y_2 = 0, \ldots, y_N = 0$ and

$$\Omega^{(3)}_{jklm} = \sum_{\substack{j',k',l' \text{ are all} \\ \text{combinations} \\ \text{of } j,k,l,m}} \phi_{j'k'l'}\phi_{m'} = \phi_{jkl}\phi_m + \phi_{mjk}\phi_l + \phi_{lmj}\phi_k + \phi_{klm}\phi_j \quad (10)$$

$$\Omega^{(2)}_{jklm} = \sum_{\substack{j',k' \text{ are all} \\ \text{combinations} \\ \text{of } j,k,l,m}} \phi_{j'k'}\phi_{l'}\phi_{m'} = \phi_{jk}\phi_l\phi_m + \phi_{jl}\phi_k\phi_m + \phi_{jm}\phi_k\phi_l + \phi_{kl}\phi_j\phi_m + \phi_{km}\phi_j\phi_l + \phi_{lm}\phi_j\phi_k$$

With reference to the differential properties of the characteristic function, namely

$$\phi^* = 1, \quad \phi^*_j = i\mu_j \quad \phi^*_{jk} = -\mu_{jk}$$
$$\phi^*_{jkl} = -i\mu_{jkl}, \quad \phi^*_{jklm} = \mu_{jklm} \quad (11)$$

it follows that at $Y = \mathbf{0}$ (10) becomes the same used by Fleming. The quasi-normal procedure also results in an identity for the 5th-order terms

$$\phi^4 \phi_{jklm} - \phi^3 \Omega^{(4)}_{jklmn} + \phi^2\Omega^{(3)}_{jklmn} - \phi\Omega^{(2)}_{jklmn} + 4\phi_j\phi_k\phi_l\phi_m\phi_n = 0 \quad (12)$$

where $\Omega^{(4)}_{jklmn}$, $\Omega^{(3)}_{jklmn}$, $\Omega^{(2)}_{jklmn}$ are determined like (10) but for five indices. Eq. (12) at $Y = \mathbf{0}$ states the 5th central moments vanish in the case of the normal distribution. Eqs. (9) and (12) are deduced by direct substitution of the Gaussian characteristic function. Therefore the terms in question can be calculated from (9) and (12), so the system of eqs. (6), (7), (9) and (12) is closed. It can be initialized by a multivariate normal distribution with independent uncorrelated variables for which

$$\phi(0; Y) = \exp\left(i \sum_p \mu_p(0)y_p - \tfrac{1}{2} \sum_p \sigma_p(0)y_p^2\right), \quad (13)$$

where $\sigma_p(0)$ denotes the variance of x_p at $t = 0$.

4. The approximate marginal density function

Now it is possible to iterate the approximate system deduced above, although the solution of the whole system would be an enormous undertaking. On the other hand we are mainly concerned with the marginal distributions of the process $X(t)$, i.e. the stochastic behaviour of the individual variables $x_1, x_2, \ldots, x_N$. Let us choose the first coordinate for the sake of simplicity. In this case the approximate system must be solved only for points $Y = (y, 0, \ldots, 0)$. Given the boundary conditions $\phi(t; Y) \to 0$ as $y \to \pm\infty$ we introduce the grid $0, \pm\varepsilon, \pm 2\varepsilon, \ldots, \pm H\varepsilon$ along the domain of y. After computing $\phi(t; Y_h)$ at any time instant t, where $Y_h = (h\varepsilon, 0, \ldots, 0)$ an estimation can be given for the probability density function of $x = x_1$ as follows

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ixy}\, \Phi(y)\, dy \approx \frac{1}{2\pi} \sum_{-H}^{H} \int_{h\varepsilon-\varepsilon/2}^{h\varepsilon+\varepsilon/2} e^{-ixy} \times \sum_{l=0}^{L} \Phi^{(l)}(h\varepsilon)(y - h\varepsilon)^l \frac{1}{l!}\, dy \quad (14)$$

where $\Phi(y) = \phi(y, 0, \ldots, 0)$, $\Phi^{(1)}(y) = \phi_1(y, 0, \ldots, 0)$, $\Phi^{(2)}(y) = \phi_{1,1}(y, 0, \ldots, 0)$ etc. For sufficiently smooth functions one can make the choice of the maximum simplified case of $H = 0$ provided L is large enough. Specifically we will assume that $L = 4$. Then it is required to solve the system (6), (7) for $y_1 = y_2 = \cdots = y_N = 0$ resulting in the following approximation for the characteristic function

$$\tilde{\Phi}(y) = 1 + i\mu_1 y - \tfrac{1}{2}\mu_{11}y^2 - \tfrac{1}{6}i\mu_{111}y^3 + \tfrac{1}{24}\mu_{1111}y^4 \quad (15)$$

Eq (15) applied to (14) allows us to give an explicit expression of the estimated density function

$$\tilde{f}(x) = \frac{1}{2\pi}(J_0 - \mu_1 J_1 - \tfrac{1}{2}\mu_{11}J_2 + \tfrac{1}{6}\mu_{111}J_3 + + \tfrac{1}{24}\mu_{1111}J_4) \quad (16)$$

where $A = \varepsilon/2$, $\alpha = \sin Ax$, $\beta = \cos Ax$ and

$$J_0 = \frac{2}{x}\alpha, \quad J_1 = \frac{1}{x}(2A\beta - J_0),$$

$$J_2 = \frac{1}{x}(2A^2\alpha + 2J_1), \quad J_3 = \frac{1}{x}(2A^3\beta - 3J_2),$$

$$J_4 = \frac{1}{x}(2A^4\alpha + 4J_3) \tag{17}$$

The l'Hopital's law, i.e. derivating the numerators and the denominators separately gives formulas in the environment of $x = 0$ because of the singularity of the expressions in (17)

$$J_0 = 2A\beta, \quad J_1 = -A^2\alpha, \quad J_2 = \tfrac{2}{3}A^3\beta,$$
$$J_3 = -\tfrac{1}{2}A^4\alpha, \quad J_4 = \tfrac{2}{5}A^5\beta \tag{18}$$

which will be used in the interval $(-B, B)$. Numerical computations indicate that for the normally distributed variable with parameters $\mu_1 = 0$, $\mu_{11} = 1$ the absolute deviation of the estimator (16)–(18) from the theoretical density function is least when setting $A = 1.73$ and $B = 0.35$. For this empirical value A the estimator (18) is more adequate within $(-B, B)$ than (15)–(16). Table 1 lists selected values of this normal density function and the approximate one.

5. Lorenz's maximum simplified dynamic equations

Lorenz (1960) succeeded in derivation of minimum hydrodynamic equations by spectral expansion of the stream-function ψ in the vorticity equation

$$\frac{\partial}{\partial t}\nabla^2\psi = -\bar{k}\cdot\nabla\psi x\nabla(\nabla^2\psi) \tag{19}$$

over a rectangular region $2\pi/k \times 2\pi/l$. The simplest approximation of the vorticity is maintained by three spectral terms

$$\nabla^2\psi = A_1\cos ly + A_2\cos kx + 2A_6\sin kx\sin lx \tag{20}$$

The evolution of the Fourier-coefficients is given by

$$\dot{A}_1 = \beta_1 A_2 A_6, \quad \dot{A}_2 = \beta_2 A_1 A_6, \quad \dot{A}_6 = \beta_3 A_1 A_2 \tag{21}$$

where $\beta_1, \beta_2, \beta_3$ are functions of $\gamma = k/l$. Taking $\gamma = 2$ one can derive that $\beta_1 = -0.1$, $\beta_2 = 1.6$, $\beta_3 = -0.75$. The dimension of the coefficients A_1, A_2, A_6 is $(\text{time})^{-1}$. Following Lorenz the time unit is 3 h while the time step of the integration is $\tau = 2$ which corresponds to 6 h. In the first situation Lorenz considered a cyclical exchange of energy between the zonal flow expressed by A_1 and the eddies, which mainly are characterized by A_2 and A_6. He took $A_1 = 0.12$, $A_2 = 0.24$ and $A_6 = 0.0$ initially. In the stochastic dynamic version the first moments of these variables will have the same values. Like Epstein's (1969) computations we now assume that in (13) $\sigma_1(0) = \sigma_2(0) = \sigma_6(0) = 10^{-4}$. At $t = 18$ h we have the following estimations for the three first central moments of A_6

$$\mu_6 = -0.12, \quad \sigma_6 = 1.86\times10^{-4}, \quad \tau_6 = 14.77\times10^{-8}$$

It is most convenient to introduce the standardized stochastic variable $\hat{A}_6 = (A_6 - \mu_6)/\sqrt{\sigma_6}$ for which

$$\hat{\mu}_6 = 0, \quad \hat{\mu}_{66} = 1, \quad \hat{\mu}_{666} = \frac{\tau_6}{\sigma_6^{1.5}} = 0.058$$

and the fourth moment can be computed by the quasi-normal assumption, $\hat{\mu}_{6666} = 3\hat{\mu}_{66}^2 = 3$. So the characteristic function of $\hat{A}_6$ is approximated by

$$\hat{\Phi}_6(y) = 1 - \tfrac{1}{2}y^2 - \tfrac{1}{6}i0.058y^3 + \tfrac{1}{8}y^4$$

from which one can get an estimation of the density function $\hat{f}_6$ of $\hat{A}_6$ applying (16). The density function of A_6 then

$$\tilde{f}_6(\mu_6 + x\sqrt{\sigma_6}) = \hat{f}_6(x)\frac{1}{\sqrt{\sigma_6}}$$

Table 1. *Selected values of the normal density function f with $\mu_1 = 0$, $\mu_{11} = 1$ and the estimation $\tilde{f}$ derived via characteristic function (functions are symmetric)*

x	f	$\tilde{f}$	x	f	$\tilde{f}$
0.0	0.40	0.40	0.5	0.35	0.36
0.1	0.40	0.39	1.0	0.24	0.26
0.2	0.39	0.38	1.5	0.13	0.14
0.3	0.38	0.37	2.0	0.05	0.04
0.35	0.38	0.37	2.5	0.01	−0.01
0.4	0.37	0.37	3.0	0.00	−0.02

Table 2. *Selected values of density function $\hat{f}_6$ of variable A_6 in Lorenz's minimum equations and density function g with no third moment at $t = 0$ and $t = 18$ h*

$t = 0$ h		$t = 18$ h					
$\mu = \mu_6 = 0.00$ $D = \sqrt{\sigma_6} = 10^{-2}$		$\mu = \mu_6 = -0.12$ $D = \sqrt{\sigma_6} = 1.36\ 10^{-2}$					
x	$\hat{f}_6 = g$	x	$\hat{f}_6$	x	$\hat{f}_6$	x	g
μ	39.9	μ	29.4	μ	29.4	μ	29.4
$\mu \pm 0.1\ D$	39.3	$\mu + 0.1\ D$	28.8	$\mu - 0.1\ D$	29.0	$\mu \pm 0.1\ D$	28.9
$\mu \pm 0.25D$	37.0	$\mu + 0.25D$	26.5	$\mu - 0.25D$	30.7	$\mu \pm 0.25D$	28.6
$\mu \pm 0.5\ D$	35.6	$\mu + 0.5\ D$	25.4	$\mu - 0.5\ D$	26.1	$\mu \pm 0.5\ D$	25.7
$\mu \pm 1.0\ D$	26.1	$\mu + 1.0\ D$	18.7	$\mu - 1.0\ D$	19.7	$\mu \pm 1.0\ D$	19.2
$\mu \pm 1.5\ D$	13.8	$\mu + 1.5\ D$	9.7	$\mu - 1.5\ D$	10.6	$\mu \pm 1.5\ D$	10.1
$\mu \pm 2.0\ D$	3.6	$\mu + 2.0\ D$	2.5	$\mu - 2.0\ D$	2.8	$\mu \pm 2.0\ D$	2.6
$\mu \pm 2.5\ D$	−1.7	$\mu + 2.5\ D$	−1.1	$\mu - 2.5\ D$	−1.4	$\mu \pm 2.5\ D$	−1.3

Table 2 lists some values of $\hat{f}_6$ and that with no third moment at $t = 0$ and $t = 18$ h. The generalization led to asymmetric density function, but the short time interval of the integration makes it impossible to estimate the rate of the asymptotical dispersion of the density. Clearly, negative values resulted from extremely finite approximation (14)–(15). Knowledge of the density function enables us, among others, to form a probability prediction. The situation treated above corresponds to the first variant of Lorenz's model, in which there is an alternating ratio of the zonal flow (A_1) and the eddies (A_2, A_6). In the generalized version such an interpretation characterizes only the mean behaviour of the system. Considering, e.g. the case of eddies dominating over the zonal flow, or simply taking into account large values of the proper coefficients, its permanent existence has also a time-independent probability. For sake of simplicity, the probability of large A_6-values can be predicted in this connection as

$$P\{A_6 > A_{\text{crit}}\} = \int_{A_{\text{crit}}}^{\infty} f_6(x)\,dx$$

$$\approx \sqrt{\sigma_6} \int_{\hat{A}_{\text{crit}}}^{\infty} \hat{f}_6(x)\,dx$$

where A_{crit} denotes an empirical threshold, $\hat{A}_{\text{crit}} = (A_{\text{crit}} - \mu_6)\sqrt{\sigma_6}$. Certainly, the comparatively dominant character of the eddies can be evaluated on the basis of the common distribution of at least A_1 and A_6. Inferences can be drawn with respect to the other future relations between the predicted variables in a similar way. By the aid of the estimated density function its various functionals are available. Especially moments and central moments, as well as conditional variances and the entropy, can be estimated for the purpose of the investigation of predictability.

6. Conclusions

The simplest method for the stochastic analysis of a dynamic model is the well-known Monte Carlo procedure. It requires numerous runs of the same model with random initial values or forcing terms of a given distribution. A similar technical effort is expected when assuming the distribution in question to be discrete. The analytical generalization is more advantageous for such a model ought to be integrated only once for a fixed distribution. On the other hand a continuous stochastic variable can be entirely characterized by its probability density function or, under regular conditions, by the characteristic function. Thus the dimensionality of the phase space of the totally extended model would be twice as much as that of the original model. Unfortunately the numerical difficulties cannot be avoided by considering only a set of the variables, since their initial uncertainty may propagate to arbitrary other variable. Nevertheless the numerical integration of the system can be fulfilled in such a way that only the fixed subspace of the variables are represented by its multivariate density function, while the rest are described with the first moments reflecting only their mean behaviour. In the particular case of a single selected variable it means the computation of the proper marginal density function. This selective description is realized by means of the probability characteristic function. In spite of this technique the numerical integration of the stochastic dynamic model treated in this paper is time-consuming with respect to the classical model. Moreover it requests further pondering upon the closure of the system and the simplest way of the approximate inverse Fourier transformation to get the density function.

The advantages of the knowledge of the predicted density function appear in two forms: (1) Probability prognosis may comprise more local maxima of the density function or a system of confidence intervals, etc. (2) Predictability of the investigated system may be followed by means of functionals being finer than and differing from the variance. All the information provided by the classical method, e.g. means, variances and covariances, may be also estimated in the generalized version. Epstein (1969) notes that the "deterministic" forecast is not wrong, but poor in comparison with the stochastic one. We can qualify the model with an estimation of the density function as a more entire solution of the problem.

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ВВЕДЕНИЕ ХАРАКТЕРИСТИЧЕСКОЙ ФУНКЦИИ В СТОХАСТИКО-ДИНАМИЧЕСКОЕ МОДЕЛИРОВАНИЕ

Характеристическая функция вероятностного распределения применена для расширения стохастико-динамической прогностической модели Эпстейна. Конечно-разностная схема по времени влечет в бесконечную систему уравнений, которая аппроксимирована с помощью т.н. квази-нормального подхода. Эта система определяет непосредственную оценку совместной или произвольной маргинальной характеристической функции, которая в свою очередь, трансформируется к некоторому приближению вероятностной функции плотности. Результаты иллюстрируются на примере минимальных гидродинамических уравнений Лоренца.