Indispensable Finite Time Corrections for Fokker-Planck Equations from Time Series Data

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The reconstruction of Fokker-Planck equations from observed time series data suffers strongly from finite sampling rates. We show that previously published results are degraded considerably by such effects. We present correction terms which yield a robust estimation of the diffusion terms, together with a novel method for one-dimensional problems. We apply these methods to time series data of local surface wind velocities, where the dependence of the diffusion constant on the state variable shows a different behavior than previously suggested.

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When dynamical phenomena involve only a few degrees of freedom, the underlying equations of motion can be estimated from time series data. Within the framework of nonlinear time series analysis [1] this has attracted large attention during recent years [2,3]. In these and many other approaches, the deterministic part of the dynamics has been in the focus of interest. Using models of different levels of sophistication, many time series data have been shown to be predictable beyond the mere effect of linear correlations.

Recently, it was suggested that also the stochastic components in the time evolution of observables might possess interesting properties and hence should be extracted from data. The idea followed in [4] is that a Fokker-Planck equation rules the time evolution of the phase space density $\rho(\vec{x}, t)$ of a process, according to

$$\dot{\rho} = -\nabla \mathbf{D}^{(1)}\rho + \nabla^2 \mathbf{D}^{(2)}\rho \,, \tag{1}$$

where the deterministic contribution $\mathbf{D}^{(1)}$ is called the drift term, and $\mathbf{D}^{(2)}$ is the diffusion tensor. The assumption of Refs. [4–7] is that a corresponding Langevin equation exists and has its solution in the individual trajectory which is represented by an observed time series:

$$\dot{\vec{x}} = \mathbf{f}(\vec{x}) + \mathbf{G}(\vec{x})\Gamma \,, \tag{2}$$

where $\vec{x} \in \mathbf{R}^d$ is the d-dimensional state vector, $\mathbf{f}$ a vector field representing the deterministic force, and $\mathbf{G}$ a $d \times n$ tensorial function on the state space governing the noise inputs. Γ is a n-dimensional Gaussian white noise process with $\langle \Gamma_k(t)\Gamma_{k'}(t')\rangle = 2\delta_{k,k'}\delta(t - t')$ following the convention of Risken [8]. If this equation is interpreted in the Stratonovich sense, Eq. (1) is the corresponding Fokker-Planck equation, with $D_i^{(1)} = f_i + G_{kj}\frac{\partial}{\partial x_k}G_{ij}$ and $D_{ij}^{(2)} = G_{ik}G_{jk}$, where the contraction eliminates the dimensionality n of the noise process. A solution of the Langevin equation contains information about both $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ which was determined in [4–7] by the following estimators:

$$\mathbf{D}^{(1)}(\vec{x}) = \lim_{\Delta\to 0}\frac{1}{\Delta}\langle \vec{x}_{t+\Delta} - \vec{x}_t\rangle_{\vec{x}} \,, \tag{3}$$

$$D^{(2)}(\vec{x})_{ij} = \lim_{\Delta\to 0}\frac{1}{2\Delta}\langle (\vec{x}_{t+\Delta} - \vec{x}_t)_i(\vec{x}_{t+\Delta} - \vec{x}_t)_j\rangle_{\vec{x}} \,, \tag{4}$$

where $\langle\cdots\rangle_{\vec{x}}$ denotes the conditional average that $\vec{x}_t = \vec{x}$. The right-hand sides of Eqs. (3) and (4) are the time series estimates of the first and second moments of the conditional probability density $P(\vec{x}, t + \Delta \,|\, \vec{x}', t)$, which in the limit of $\Delta \to 0$ are shown to yield $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ in [8]. Hence, in an elegant way $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ can be estimated also in situations where the time series does not represent a stationary density $\rho(\vec{x}, t) = \rho(\vec{x})$.

The rather evident contamination of the estimated diffusion terms in [5–7] with contributions from the squares of the drift terms suggests that in applications of this method to data sets stemming from hydrodynamic turbulence and stock markets the convergence for $\Delta \to 0$ of the numerical estimates based on Eqs. (3) and (4) has not been checked and that, in fact, non-negligible corrections have to be employed in order to get reliable estimates of $\mathbf{D}^{(2)}$ from time series data with finite Δ. Taking for granted that Δ in a time series is sufficiently small to represent properly the limit, one can find diffusion terms whose state dependences are mere artifacts, as we will show below. The drift terms, however, can be rather safely estimated by Eq. (3) [9].

In the remainder of this paper we present the novel finite Δ corrections for a robust estimate of $\mathbf{D}^{(2)}$, we propose a Fokker-Planck based new estimate for one-dimensional problems, and we illustrate these findings by numerical examples. Finally, we apply the method to field measurements of surface wind velocities, thereby demonstrating that substantial corrections to the previously published results on turbulence arise from the application of our method.

Let a time series of state space observations $\{\vec{x}_t, t = 1, \ldots, T\}$ with a temporal spacing Δ (also called the sampling interval) be the solution of the Langevin equation (2). In the following we will restrict ourselves to a one-dimensional state space, but the generalization is straightforward when not otherwise said. If we are not explicitly assuming that the state space density ρ has reached its asymptotic, time invariant limit, we cannot employ the ergodic theorem in order to convert the time series into the density ρ. Hence, without this assumption, we have to consider explicitly the time evolution of a different rather than the full state space density. In fact, the transition probability $P(x, \Delta \mid x_0, 0)$ is time invariant. For small Δ it reads [8]

$$P(x, \Delta \mid x_0, 0) = \frac{1}{\sqrt{4\pi \mathbf{D}^{(2)}(x_0)\Delta}}\, e^{-\frac{[x - x_0 - \mathbf{D}^{(1)}(x_0)\Delta]^2}{4\mathbf{D}^{(2)}(x_0)\Delta}}. \qquad (5)$$

Computing its second moment for nonvanishing Δ yields the following improved estimate of $\mathbf{D}^{(2)}$:

$$\mathbf{D}^{(2)} \approx \frac{1}{2\Delta}[\langle(\vec{x}_{t+\Delta} - \vec{x}_t)(\vec{x}_{t+\Delta} - \vec{x}_t)^\dagger\rangle_{\vec{x}} - \Delta^2 \mathbf{D}^{(1)}\mathbf{D}^{(1)\dagger}]. \qquad (6)$$

Depending on the relative magnitude of drift and diffusion and on the value of Δ, the estimate of $\mathbf{D}^{(2)}$ can become fairly bad if one ignores the existence of the rightmost term of Eq. (6). This correction takes into account that a bundle of trajectories emerging from $x(t = 0) = x_0$ spreads according to $\sqrt{\Delta \mathbf{D}^{(2)}}$, but simultaneously experiences a displacement proportional to Δ due to the drift. Consequently, for infinitesimal Δ, Eq. (4) is recovered. For finite Δ, Eq. (4) is strongly biased by the square of the drift term.

The numerical example presented below shows that this is not the only correction to $\mathbf{D}^{(2)}$ of order Δ. The second relevant correction is a nonlocal effect. Imagine starting the previously mentioned bundle of initial conditions exactly on the barrier of a double well potential: as soon as this packet starts to spread out due to the diffusion, the trajectories on either side of the potential barrier begin to experience a drift towards the potential minima, thus enhancing diffusion, but leaving the mean value of this sample unchanged. Exactly the opposite phenomenon of suppressed diffusion occurs at a potential minimum. These are of cause finite Δ effects. Intuitively, the curvature of the potential should introduce a correction to the diffusion term.

We hence have to discuss the finite time solution of the Fokker-Planck equation, where the initial condition is a δ peak at $\vec{x}_0$. Introducing the abbreviation $D^{(1)\prime} := d/dx D^{(1)}(x)$, it is straightforward to verify that

$$\rho(x, \Delta) = \frac{e^{-\frac{[x - x_0 - D^{(1)}(x_0)\Delta]^2}{4D^{(2)}\Delta[1 + \Delta D^{(1)\prime}(x_0)]}}}{\sqrt{4\pi D^{(2)}(x_0)\Delta[1 + \Delta D^{(1)\prime}(x_0)]}} \qquad (7)$$

satisfies this initial condition, it conserves total probability, and inserted into the Fokker-Planck equation it cancels the $\mathbf{D}^{(1)\prime}\rho(x)$ term, which survives when doing the same with Eq. (5) [10]. The correction factor $1 + \Delta D^{(1)\prime}$ can, as expected, enhance or suppress diffusion, depending on the sign of the derivative of the drift term. One evident limit for the validity of this approximation is $\Delta D^{(1)\prime}(x_0) \ll -1$.

In the numerical scheme, one computes the estimates of $\mathbf{D}^{(1)}(x)$ and its numerical derivative with respect to x, the latter most conveniently after fitting a smooth curve to the empirical values of $\mathbf{D}^{(1)}$. Then the following estimate for the diffusion term holds for short but finite Δ:

$$D_{ij}^{(2)} = \frac{[\langle(\vec{x}_{t+\Delta} - \vec{x}_t)_i(\vec{x}_{t+\Delta} - \vec{x}_t)_j\rangle_{\vec{x}} - \Delta^2 D_i^{(1)}(\vec{x}) D_j^{(1)}(\vec{x})]}{2\Delta\left(1 + \Delta \frac{dD_i^{(1)}(\vec{x})}{dx_j}\right)}. \qquad (8)$$

Since the prefactor Δ of the derivative of $\mathbf{D}^{(1)}$ cancels the Δ in the normalization of $\mathbf{D}^{(1)}$, the knowledge of Δ in physical units is not required for a correct estimate of $\mathbf{D}^{(2)}$, both $\mathbf{D}^{(2)}$ and $\mathbf{D}^{(1)}$ can be measured in arbitrary temporal units.

We demonstrate the need for our corrections and their accuracy employing the example of [4]. An overdamped particle in a double well potential with stochastic inputs is described by the Langevin equation

$$\dot{x} = 0.1x - x^3 + a\Gamma, \qquad (9)$$

where Γ is again white noise. The drift and diffusion terms of the corresponding Fokker-Planck equation (where Ito and Stratonovich calculi are equivalent) read $D^{(1)}(x) = 0.1x - x^3$ and $D^{(2)}(x) = a^2$. Figure 1 shows the different estimates of the diffusion term, together with the drift term, for $\Delta = 0.5$. Evidently, without correction, the diffusion constant seems to have a complicated space dependence, one part of which is the square of the drift term. After proper subtraction of the latter, however, the factor $1 + \Delta \frac{d}{dx} D^{(1)}$ is needed for a correction of comparable magnitude.

In one-dimensional problems we suggest an alternative method to calculate $D^{(2)}(x)$ by exploiting the Fokker-Planck equation directly: If the time series represents an invariant density, this implies $\dot{\rho} = 0$ and hence

$$\int_{-\infty}^{x} \frac{d}{dx'} D^{(1)}(x')\rho(x')\,dx' = \int_{-\infty}^{x} \frac{d^2}{dx'^2} D^{(2)}(x')\rho(x')\,dx'. \qquad (10)$$

If $\rho(x)$ decays exponentially and drift and diffusion behave algebraically, the integrals vanish at their lower limits. Estimating the drift term as before and the density $\rho(x)$ in a straightforward way allows one to determine the diffusion term through the numerical evaluation of

$$D^{(2)} = \frac{\int_{-\infty}^{x} D^{(1)}(x')\rho(x')\,dx'}{\rho(x)}, \qquad (11)$$

if we assume again that $D^{(2)}(-\infty)\rho(-\infty) = 0$. Let us point out that here the temporal sampling interval Δ enters only through the accuracy of the estimate of the drift term $D^{(1)}$; hence this method is particularly suited for large Δ.

For the motion in the double well from above, we find the results depicted in Fig. 2 for the diffusion term, for the same Δ as before. They agree very well with the given $D^{(2)}$.

Following the pioneering work of [5,6], we now apply our new corrections in a different setting, namely to data from turbulence and their scale dependence. Let us analyze the scale-to-scale evolution of the distribution $P(u_r)$ of

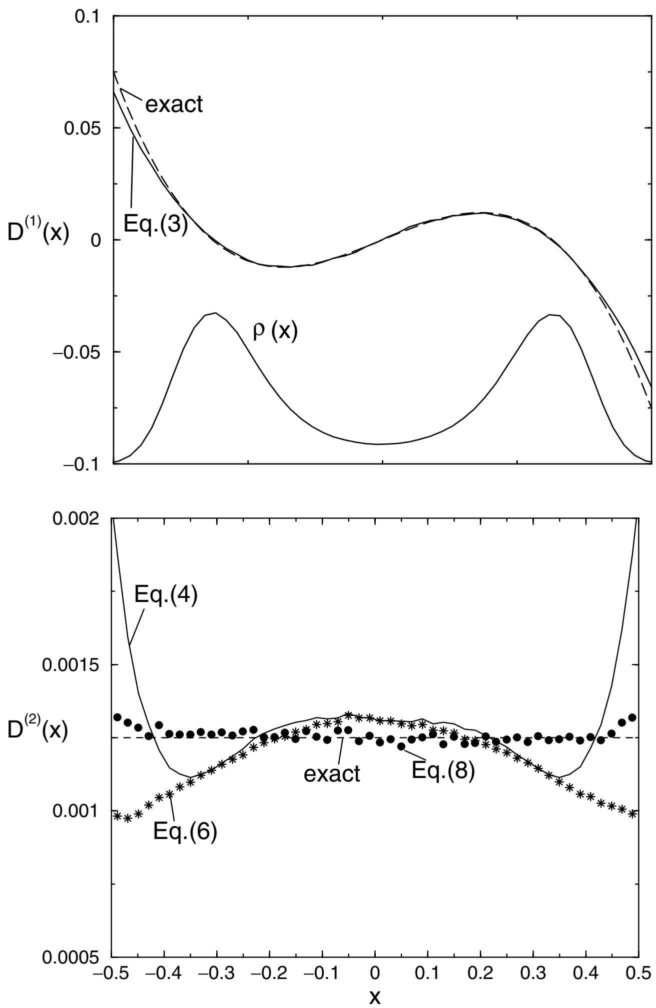

FIG. 1. Drift term [upper panel, together with the invariant density $\rho(x)$] and diffusion term (lower panel) obtained from time series data of Eq. (9). While the drift term is estimated reasonably well for this sampling rate $\Delta = 0.5$, the estimate of Eq. (4) yields a false space dependence of the diffusion term, which is successfully corrected by Eq. (8).

velocity increments $u_r(x) = u(x + r) - u(x)$. It was found in [5] that the r evolution of the distribution can be described by a Markov process. The Markovian property has been evaluated by the investigation of conditional probabilities $P(u_{r_2}, r_2 \,|\, u_{r_1}, r_1)$, with $r_2 < r_1$. The stochastic dynamics has been estimated from measured data applying the following procedure: First the Markovian property was checked by evaluating the Chapman-Kolmogorov equation for the $P(u_{r_2}, r_2 \,|\, u_{r_1}, r_1)$:

$$P(u_{r_2}, r_2 \,|\, u_{r_1}, r_1) = \int_{-\infty}^{\infty} P(u_{r_2}, r_2 \,|\, u_{r'}, r') \times P(u_{r'}, r' | u_{r_1}, r_1)\, du_{r'} . \quad (12)$$

Then a Fokker-Planck equation was set up as

$$-\frac{\partial}{\partial r} P(u_r, r) = \left(-\frac{\partial}{\partial u_r} D^{(1)}(u_r, r) + \frac{\partial^2}{\partial u_r^2} D^{(2)}(u_r, r) \right) \times P(u_r, r) , \quad (13)$$

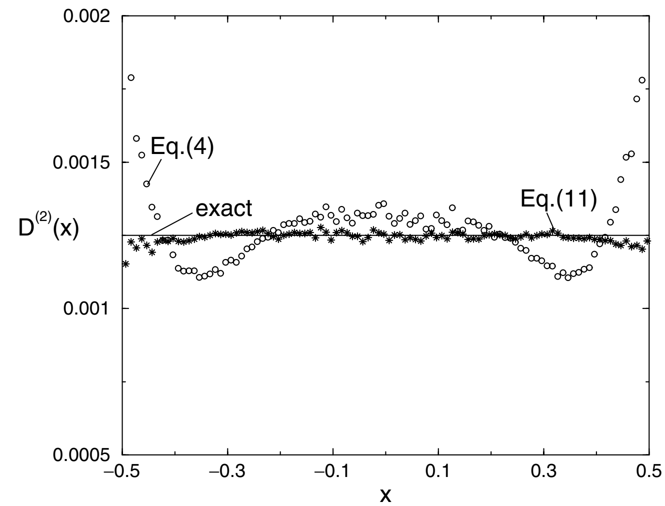

FIG. 2. The estimate of $D^{(2)}(x)$ from Eq. (11).

with coefficients defined in accordance with Eq. (4)

$$D^{(k)}(u_r, r) := \lim_{\delta \to 0} M^{(k)}(u_r, r, \delta) ,$$
$$M^{(k)}(u_r, r, \delta) := \frac{1}{k!} \frac{1}{\delta} \int (u_{r'} - u_r)^k \times P(u_{r'}, r' \,|\, u_r, r)\, du_{r'} , \quad (14)$$

where $\delta = r - r'$. We will follow this procedure, but apply our corrections.

We use data of atmospheric surface wind velocities recorded on the Lammefjord on the island Seeland in Denmark. The terrain around the measurement station is very flat and no major obstacles interfere with the fluid flow. One component of the wind velocity was recorded with a sampling rate of 16 Hz using an ultrasonic anemometer located at an altitude of 40 m during a period of 24 h. A typical time series of the wind velocity is shown in Fig. 3. Using the method of extended self-similarity [11] the structure functions up to order five where estimated and the calculated scaling exponents show reasonable agreement with the expected values for three-dimensional turbulence. Also the power spectrum obeys the expected $(-5/3)$ scaling behavior. In this sense our time series are a "good" representative for fully developed turbulence. In Fig. 4 the probability density functions (pdf's) $P(u_r)$ of $u_r(x)$ are shown. We observe the well known intermittency effect of isotropic turbulence; i.e., we find exponential

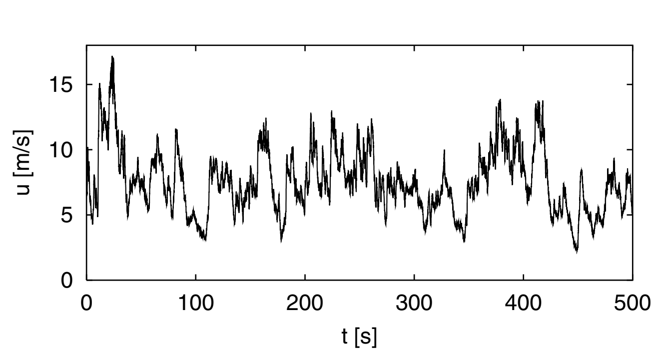

FIG. 3. Part of the wind data used.

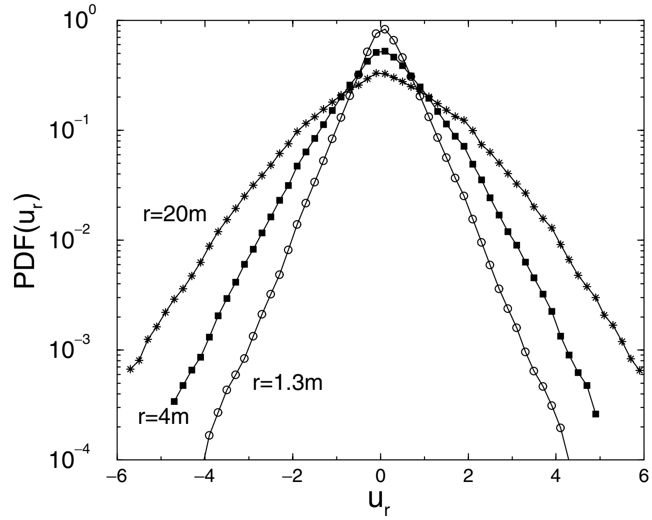

FIG. 4. PDF for different separations r.

behavior at small scales and almost Gaussian behavior at large scales. We have checked the Chapman-Kolmogorov equation in Fig. 5 and found reasonable agreement, hence confirming the Markov property of fully developed turbulence. As a last step, we calculated the drift and diffusion coefficients. The drift coefficient shows a linear behavior in agreement with [5]. In Fig. 6 we compare the estimates of the diffusion coefficients obtained with Eq. (4) to our improved estimates Eq. (8). We find a significantly shallower slope of the corrected graphs. If one assumes a quadratic behavior of $D^{(2)}(u_r) = \alpha + \beta u_r + \gamma u_r^2$ as done in Renner *et al.* [12], one hence obtains important corrections for β and γ. Actually, Renner *et al.,* by integrating the Fokker-Planck equation using their fitted values of $D^{(2)}$, report already that their method yields too large values for β and γ.

In summary, from an improved expression for the transition probability $P(\vec{x}', t + \Delta \mid \vec{x}, t)$ for finite Δ, we obtain

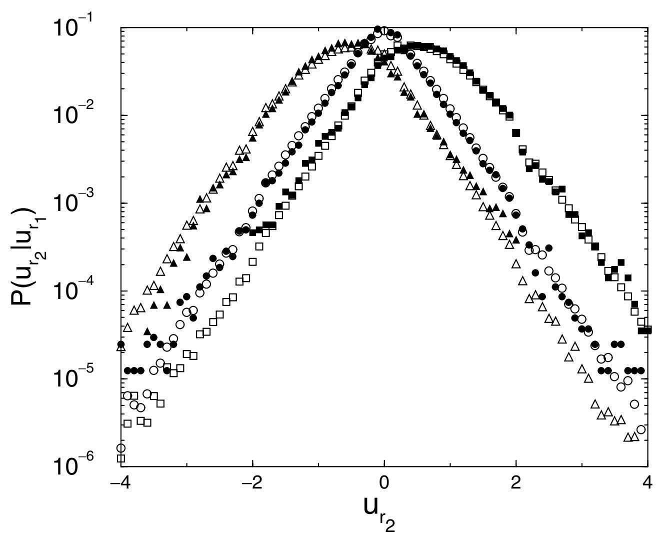

FIG. 5. Test of the Chapman-Kolmogorov equation for different values of $u_{r_1} = -1m/s; 0m/s; 1m/s$; bold symbols represent directly evaluated pdf, open symbols integrated pdf.

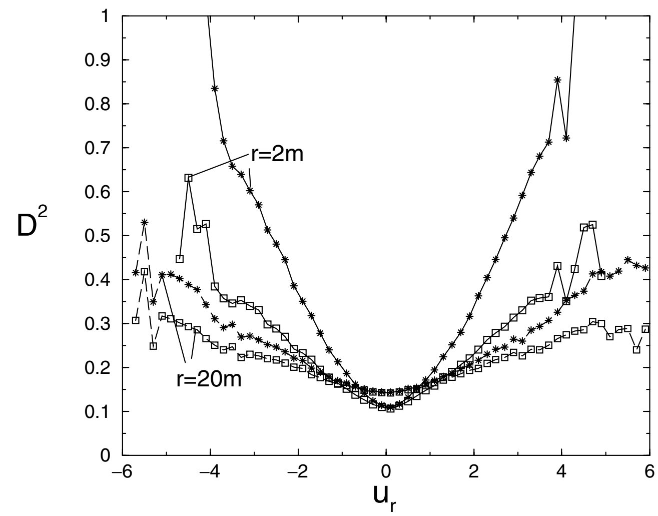

FIG. 6. Diffusion coefficient for different separations r; stars correspond to the naive method and squares to the corrected estimate.

an important correction for the estimate of the diffusion term in a Fokker-Planck equation from time series data, whose relevance is evidenced by a numerical example and by surface wind velocity data.

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