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Validation of drift and diffusion coefficients from experimental data

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Abstract. Many fluctuation phenomena, in physics and other fields, can be modeled by Fokker–Planck or stochastic differential equations whose coefficients, associated with drift and diffusion components, may be estimated directly from the observed time series. Its correct characterization is crucial to determine the system quantifiers. However, due to the finite sampling rates of real data, the empirical estimates may significantly differ from their true functional forms. In the literature, low-order corrections, or even no corrections, have been applied to the finite-time estimates. A frequent outcome consists of linear drift and quadratic diffusion coefficients. For this case, exact corrections have been recently found, from Itô–Taylor expansions. Nevertheless, model validation constitutes a necessary step before determining and applying the appropriate corrections. Here, we exploit the consequences of the exact theoretical results obtained for the linear–quadratic model. In particular, we discuss whether the observed finite-time estimates are actually a manifestation of that model. The relevance of this analysis is put into evidence by its application to two contrasting real data examples in which finite-time linear drift and quadratic diffusion coefficients are observed. In one case the linear–quadratic model is readily rejected while in the other, although the model constitutes a very good approximation, low-order corrections are inappropriate. These examples give warning signs about the proper interpretation of finite-time analysis even in more general diffusion processes.

Keywords: stochastic particle dynamics (experiment), stochastic particle dynamics (theory), stochastic processes, diffusion

Contents

1. Introduction

The dynamics of many natural and man-made complex systems exhibits an interplay of processes at different scales. The large-scale modes of the dynamics are usually identified with deterministic forcing (drift), while the small-scale modes, are described by recourse to stochastic terms (diffusion). In many strategic fields such as medical and biological sciences, meteorology or social-economic systems, the correct characterization of such modes is crucial.

For instance, in the biomedical domain, key aspects of brain dynamics are not captured when focusing only the slowly varying deterministic components. Analysis of electroencephalographic signals [1] indicates that it is precisely the stochastic dynamical part that allows one to discriminate between physiological and pathological activities.

Another example, in the realm of ecosystems, is the formation and maintenance of cirrus clouds. Besides the large-scale synoptic conditions in which the cirrus develop, there are small-scale processes whose variability is due to different formation mechanisms that can be regarded as noise [2]. Due to their upmost position in the atmosphere, the cirrus clouds are critical components of the Earth's climate, and therefore proper meteorological predictions call for their accurate modeling.

Comprising man-made complex systems, a prototypical example is the financial market, constituted of many agents conditioned by diverse sources of information. The resulting cooperative behavior is driven by the slow varying large-scale aggregated market information as well as by unforeseen fast varying private information. The analysis of both components is necessary for characterizing the dynamics of important market quantifiers, as for instance, risk.

As illustrated in the above examples, in such complex systems the correct quantitative estimates of the deterministic and stochastic components is a central issue once their first-principles dynamics equations are not unknown. Therefore, it is useful to resort to data-driven analysis to find a quantitative description.

For the important class of Markovian processes, which we consider here, the Kramers–Moyal expansion is the general evolution equation for the conditional probability, which completely defines a Markov process. Accordingly, the estimation of drift and diffusion coefficients from their primary definition seems a very natural procedure to obtain them from empirical data analysis. Namely, given a time series $\{X_t\}$ assumed Markovian, the time evolution for the conditional probability density function (PDF) $P(x,t|x_0,0) \equiv P(X_t = x|X_0 = x_0)$ can be described by a general evolution equation: the Kramers–Moyal (KM) expansion $\partial_t P = \sum_{k\geq 1}(-1)^k \partial_x^k (D_k P)$ [3]. The kth-order KM coefficients D_k can be numerically computed from the finite-time conditional moments:

$$\tilde{D}_k(x,\tau) = \frac{1}{k!\tau}\langle [X_{t+\tau} - X_t]^k\rangle|_{X_t=x}, \tag{1}$$

with $\langle\cdots\rangle$ denoting statistical average and $|_{X_t=x}$ meaning that at time t the stochastic variable takes the value x. The KM coefficients are obtained by estimating the limit

$$D_k(x) = \lim_{\tau\to 0} \tilde{D}_k(x,\tau). \tag{2}$$

Here we have assumed stationarity, hence suppressing the time dependence from the coefficients. The first term of the KM expansion, given by the drift coefficient $D_1(x)$, represents all slow deterministic processes in the dynamics of the system. The second term represents the stochastic approximation to the fast processes, with the diffusion coefficient $D_2(x)$ controlling the strength of the noisy force. If higher-order coefficients vanish, one obtains the special case corresponding to a Fokker–Planck equation (FPE), which can be associated, for instance, with the univariate Itô-stochastic differential equation (SDE):

$$\mathrm{d}x = D_1(x)\,\mathrm{d}t + \sqrt{2D_2(x)}\,\mathrm{d}W_t \tag{3}$$

where W_t is a standardized Wiener process.

Generalized Langevin equations (with a memory kernel like in the Mori–Kubo equation, or with correlated noise, or even dependent on non-integer moments) can also describe many dynamical processes. Here, we restrict our analysis to Markovian dynamics ruled by equation (3). Moreover, although our discussion is based on the one-dimensional case, a picture similar to the one discussed here is expected to apply in higher dimensions.

In any case, real data are constrained to finite sampling intervals and therefore one can assess directly only up to a minimal-τ estimate, which may significantly differ from the actual quantity one is looking for. This is particularly relevant when τ is not very small compared to the characteristic timescales of the process. To tackle this issue, there have been efforts in the literature to obtain corrections to finite-time estimates of KM coefficients [4]–[6]. However, different proposed low-order analytical corrections and $\tau \to 0$ extrapolation schemes led to controversies [6, 7] about the true limit D_k. This problem has been solved in a recent paper [8] for an important class of diffusion models with linear drift and quadratic diffusion terms. There, we have derived exact formulae that connect the empirical discrete-time estimates with the actual values. Notice that the addressed class of processes is frequently encountered for a diversity of systems, in physics [9, 10] as well as in other fields, such as medical [1, 11], atmospheric [2, 6, 12] or financial systems [13, 14]. The ubiquity of such simple linear and quadratic forms should not be surprising as soon as they represent a low-order approximation to generic forms of each component.

In the present work, we exploit the exact results as a framework for such data-driven analysis. As a general outcome, we discuss criteria that allow model validation, that is, to determine whether the commonly found empirical (finite-time) linear and quadratic forms are actually a consequence (or not) of the linear–quadratic model. In particular, we analyze the significance of the results according to the relation between the resolution time

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and the correlation time τ_c. For instance, as we will show below, arbitrary functional forms of drift and diffusion coefficients approach specific linear and quadratic forms, respectively, in the limit of independence, that is, as τ becomes much larger than any characteristic timescale. Then, the implications of our present results go far beyond the linear–quadratic model.

The relevance of our approach is shown by the investigation of two contrasting real data examples: one in which the linear–quadratic model is readily rejected and another in which the model constitutes a very good approximation. In the latter case, low-order corrections are not enough and the exact (infinite-order) corrections were successfully applied to recover the intrinsic hidden values.

2. Empirical assessment of linear drift and quadratic diffusion coefficients

Two exemplary real time series, one from human physiology [15] and another from finance, were considered as test cases.

The stride intervals of human walking are known to present complex fluctuations [15]. Data of long-term recordings of the stride intervals of both constrained and unconstrained walking at different rates (slow, normal, fast) are available [15]. Now we have revisited the fluctuation analysis from the present perspective. We analyzed the logarithmic increments of consecutive stride intervals of unconstrained normal walking (approx. 3000 data points). Increments were considered instead of the original series because of its stationarity. We set $\tau = 1$ as the interval between successive data.

We also considered the time series of the returns (logarithmic increments) of the Brazilian stock index Ibovespa, in the period from 1 November 2002 to 19 July 2006. Returns, computed at a 4 min timelag, without overlap, were normalized by its standard deviation (approx. 8×10^5 return values). In this case, we set 4 min as the unit of time ($\tau = 1$).

In both cases, Markovianity was checked by means of the Chapman–Kolmogorov equation [3], for the lowest available timescale, resulting in a good approximation.

Examples of the first two finite-time coefficients, given by equation (1) for each time series, are depicted in figures 1 and 2, respectively. In these examples, the finite-time drift and diffusion coefficients follow linear and quadratic forms, respectively.

We are concerned with the empirical evaluation of unknown drift and diffusion coefficients. If a theoretical ansatz for the functional dependence of the true coefficients is given, then deviations of the finite-τ estimates can be evaluated from the stochastic Itô–Taylor expansion of equation (3) [3]. Otherwise, as a first educated guess, one may assume that the coefficients have the same functional dependence found for their respective finite-τ estimates. In such a case, the empirical findings illustrated in figures 1 and 2 suggest $D_1(x) = -a_1 x$ and $D_2(x) = b_0 + b_2 x^2$, which define the model we call linear–quadratic (including state-independent diffusion). If higher-order coefficients vanish, an SDE (3) associated with the FPE is $\dot{x} = -a_1 x + \sqrt{2b_0 + 2b_2 x^2}\eta_1(t)$ or equivalently, the linear additive–multiplicative stochastic differential equation [16] $\dot{x} = -a_1 x + \sqrt{2b_0}\eta_1(t) + \sqrt{2b_2}x\,\eta_2(t)$, where $\eta_1(t)$ and $\eta_2(t)$ are (uncorrelated) zero-mean white noises with unitary variance. By applying the stochastic Itô–Taylor expansion for this class of processes, it has been shown [8] that the finite-τ coefficients preserve their functional forms. This is an important finding that legitimates the initial guess. Furthermore, it

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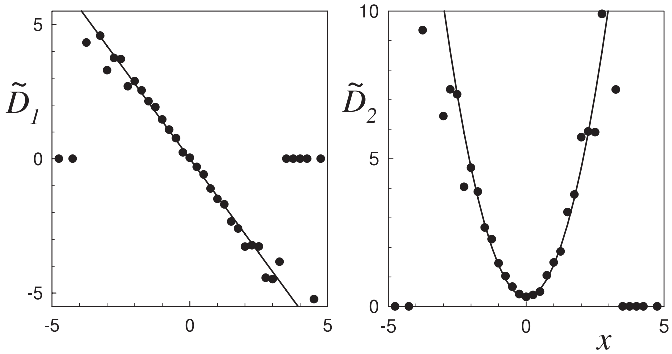

Figure 1. Coefficients $\tilde{D}_1$ (a) and $\tilde{D}_2$ (b) obtained for the (normalized) logarithmic increments of a typical time series of normal walking stride intervals [15]. Solid lines correspond to linear and quadratic least-squares fits, furnishing $(\tilde{a}_1, \tilde{b}_0, \tilde{b}_2)\tau = (1.39 \pm 0.04, 0.30 \pm 0.02, 1.08 \pm 0.03)$. The time unit $\tau = 1$ corresponds to 1 s.

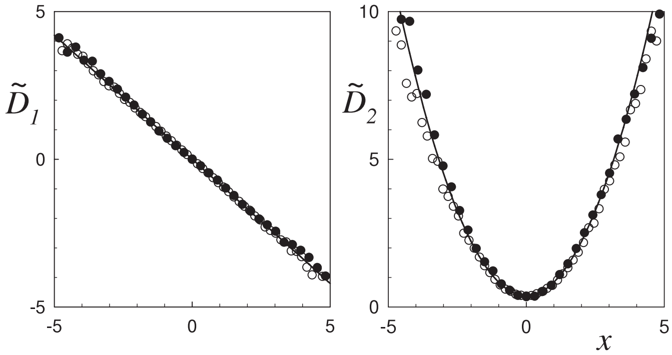

Figure 2. Coefficients $\tilde{D}_1$ (a) and $\tilde{D}_2$ (b) for normalized 4 min returns of stock index Ibovespa (filled symbols). Solid lines correspond to linear and quadratic least-squares fits, furnishing $(\tilde{a}_1, \tilde{b}_0, \tilde{b}_2)\tau = (0.84 \pm 0.03, 0.38 \pm 0.02, 0.46 \pm 0.02)$. The time unit $\tau = 1$ corresponds to 4 min. The same finite-τ coefficients computed for an artificial times series generated with the estimated coefficients D_1 and D_2, with $(a_1, b_0, b_2)\tau = (1.83 \pm 0.19, 0.71 \pm 0.08, 1.12 \pm 0.27)$ (hollow symbols).

allows the achievement of the hidden parameters (a_1, b_0, b_2) from their finite-τ counterparts $(\tilde{a}_1, \tilde{b}_0, \tilde{b}_2)$.

Let us summarize the main theoretical expressions [8]. For normalized data (with unitary variance $\sigma = 1$, hence $b_0 + b_2 = a_1$), one has

$$\tilde{a}_1(\tau) = a_1 \sum_{j\geq 0} \frac{[-a_1\tau]^j}{(j+1)!} = \frac{1 - \mathrm{e}^{-a_1\tau}}{\tau}, \quad (4)$$

$$\tilde{b}_0(\tau) = b_0 \sum_{j\geq 0} \frac{[-2b_0\tau]^j}{(j+1)!} = \frac{1 - \mathrm{e}^{-2b_0\tau}}{2\tau} \quad (5)$$

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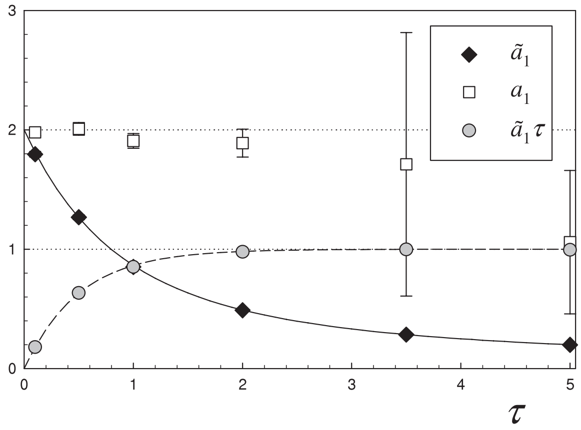

Figure 3. Dependence of finite-τ parameter $\tilde{a}_1$ on the time resolution τ (black diamonds), obtained from an artificial series with parameters $(a_1, b_0, b_2) = (2, 1, 1)$. Also plotted are $\tilde{a}_1\tau$ (gray circles) and a_1 obtained from equations (6) and (7) (white squares). Error bars were obtained from error propagation of the deviation (within symbol size) of fitting parameter $\tilde{a}_1$. Full and dashed lines correspond to the theoretical expressions obtained from equation (4). Dotted lines are drawn as reference of the upper bound of $\tilde{a}_1\tau$ and of the exact value of a_1.

and $\tilde{b}_0 + \tilde{b}_2 = \tilde{a}_1$ (thus the fluctuation–dissipation relation also holds for the finite-time parameters). If data were not normalized, the parameters b_0 and $\tilde{b}_0$ must be simply divided by σ^2. By inversion, the exact values can be obtained through

$$-a_1\tau = \ln(1 - \tilde{a}_1\tau), \tag{6}$$

$$-2b_0\tau = \ln(1 - 2\tilde{b}_0\tau). \tag{7}$$

Let us remark that equation (4) is valid for arbitrary D_2, that is, it is not restricted to the linear–quadratic model, whilst equation (5) arises from the linearity of D_1.

In figure 3 we show the dependence of the measured parameter $\tilde{a}_1$ on the resolution τ, for an artificial series generated with $(a_1, b_0, b_2) = (2, 1, 1)$. The results are well represented by equation (4). From equations (6) and (7), it is clear that $\tilde{a}_1\tau$, $2\tilde{b}_0\tau < 1$ must hold. The limits are attained when the resolution τ exceeds the characteristic timescales of the dynamics, as illustrated in figure 3 for the drift parameter. There, the upper bound for $\tilde{a}_1\tau$ is approached as $\tau \to 1/a_1$. Moreover, in principle, equations (6) and (7) would allow us to recover a_1 and b_0 for whatever resolution τ. However, error propagation leads to $\Delta a_1 = \Delta\tilde{a}_1/(1 - \tilde{a}_1\tau)$ and $\Delta b_0 = \Delta\tilde{b}_0/(1 - 2\tilde{b}_0\tau)$, implying that the deviations of the true parameters diverge as τ increases. Hence, larger τ would not only enhance uncertainties, as expected, but may also lead to wrong estimates, as shown in figure 3.

From a theoretical perspective, the upper bound is associated with the limit of independence, in which $P(x', t + \tau|x, t) = P(x', t + \tau)$. Thus

$$\tilde{D}_k(x, \tau) = \frac{1}{k!\tau}\int \mathrm{d}x'\, P(x')[x' - x]^k. \tag{8}$$

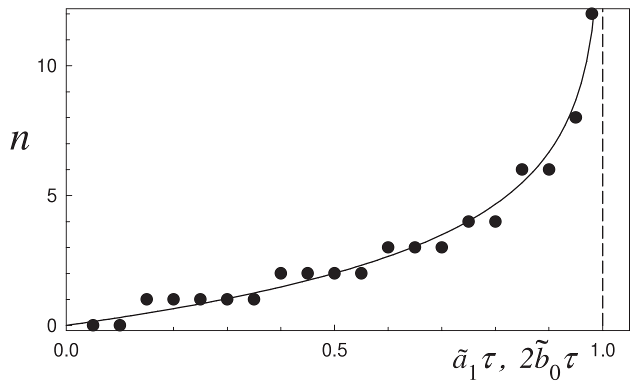

Figure 4. Dependence of the order n of the correction necessary to obtain the limiting values of the parameters within the $\pm 5\%$ interval, as a function of $\tilde{a}_1\tau$ (or $2\tilde{b}_0\tau$). The solid line is a guide to the eyes and the vertical dashed line indicates the upper bound. Notice the super-linear increase of n for values above 80% of the upper bound.

Therefore, for standardized data, one obtains

$$\tilde{D}_1(x,\tau) = -\frac{x}{\tau} \qquad \text{and} \qquad \tilde{D}_2(x,\tau) = \frac{1+x^2}{2\tau}. \tag{9}$$

This means that, in the limit of large τ, linear and quadratic finite-time coefficients with $\tilde{a}_1\tau = 1$ and $\tilde{b}_0\tau = \tilde{b}_2\tau = 1/2$ are the universal forms of $\tilde{D}_1$ and $\tilde{D}_2$ for any intrinsic D_1 and D_2. As a consequence, when the extreme values are approached, the uncertainty about the proper functional form signals the lost of significance of the results.

Equations (4) and (5) also contain the information on the nth-order correction expressions for a_1 and b_0, by inversion of the series truncated at order n. In figure 4 we plot the order n necessary to obtain the exact values of the parameters (within the $\pm 5\%$ interval), as a function of $\tilde{a}_1\tau$ (or $2\tilde{b}_0\tau$), assuming their values are precise. Notice that, even in this case, the required order n diverges as $\tilde{a}_1$ and $\tilde{b}_0$ approach their upper bound values, thus making low-order corrections unsuitable. The divergent behavior is a manifestation that the recording time τ is too large to obtain meaningful information.

3. Validation procedure and its application to real data examples

Let us outline the steps to validate the linear–quadratic model and extract the intrinsic coefficients from the knowledge of their finite-τ estimates. After checking the Markov property, computing the finite-τ coefficients $\tilde{D}_1$ and $\tilde{D}_2$ for normalized data, and obtaining the finite-τ parameters from least-squares fits to the expressions $\tilde{D}_1(x) = -\tilde{a}_1 x$ and $\tilde{D}_2(x) = \tilde{b}_2 x^2 + \tilde{b}_0$, we should perform the following checks.

(i) A first check is to verify if $\tilde{a}_1\tau < 1$. This condition must hold whenever the drift is of the form $D_1 = -a_1 x$. Otherwise, it would be a signature that the model fails. When $\tilde{a}_1\tau < 1$, one can employ equation (6) to unbury the intrinsic value a_1.

(ii) If besides D_1 being linear, D_2 is quadratic, then it must hold $2\tilde{b}_0\tau < 1$ (for unitary variance). This additional condition will allow us to obtain the intrinsic value b_0 by means of equation (7).

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(iii) If the two precedent inequalities are verified, b_2 can also be calculated from the fluctuation–dissipation relation. The constraint $\tilde{a}_1 = \tilde{b}_2 + \tilde{b}_0$ must also hold for finite-time parameters.

(iv) The linear–quadratic modeling requires vanishing higher-order coefficients, but on the basis of the Pawula theorem (which states that $D_4 = 0$ guarantees $D_k = 0$ for $k \geq 3$) [3], it is enough to analyze the fourth-order coefficient. However, since finite-τ estimates are generically non-null, it is necessary to check if this deviation originates from finite-τ effects. The comparison of the empirical $\tilde{D}_4$ with the corresponding analytical finite-τ prediction provides this indispensable check to validate the linear–quadratic modeling. In the particular case of null b_2 (Ornstein–Ulhenbeck process), an exact expression is available for $\tilde{D}_4(x, \tau)$ [8], which can be directly compared to numerical estimates. Otherwise, if b_2 is significantly non-null, this check can be performed by comparing the empirical result with $\tilde{D}_4(x, \tau)$ of artificial series, generated through equation (3), with the exact parameters extracted from equations (6) and (7).

Naturally, in general, the proposed methodology applies only beyond a minimal Markovian timescale.

Let us apply the above checks to our two test time series. The results of computing the first KM coefficients and performing linear and quadratic fits, of the forms here considered, are shown in figures 1 and 2, respectively. Let us proceed with step (i).

For the stride dynamics, the result shown in figure 1 might lead us to naively conclude that the drift is linear. However notice that $\tilde{a}_1\tau > 1$, thus forbidding the calculation of a_1. This means that the model fails, in particular, that the drift is not of the linear form here considered. Also, it might be that the Markov property was not strictly valid. Actually, in this case, the model is not expected to apply because of the non-trivial correlations previously observed in gait dynamics [15], with anti-correlated increments, while the linear–quadratic model yields exponentially decaying correlations. As this counter-example shows, the emergence of linear and quadratic forms from finite-time analysis is not exclusive of the linear–quadratic model. Therefore, it would be interesting to look more closely if some cases in which linear and quadratic coefficients were also found belong to this class of counter-examples too.

The outcomes of financial index returns, shown in figure 2, give $\tilde{a}_1\tau < 1$, $2\tilde{b}_0\tau < 1$ and $\tilde{a}_1 = \tilde{b}_2 + \tilde{b}_0$ within error bars, allowing the calculation of the limiting parameters. Furthermore, according to figure 4, the values obtained for finite-time parameters require at least a fourth-order correction. Then, contrary to the assertion in [6], the drift term cannot be safely extracted from the finite-time estimate unless τ is sufficiently small. In the present case application of equations (6) and (7) is useful, yielding the values indicated in the caption of figure 2. Artificial series generated with those values reproduce the empirical results of the first and second coefficients, as shown in figure 2.

Then, for this example it is worth considering step (iv) and compare the finite-time fourth-order coefficient for real and synthetic data. As exhibited in figure 5, the outcome of artificial series is very close to the empirical one, supporting that its non-null character can be attributed to finite-τ deviations, thus sustaining the FPE description.

One can proceed with extra checks by performing statistical analysis of the distributions and correlations predicted by the theoretical model and comparing them with

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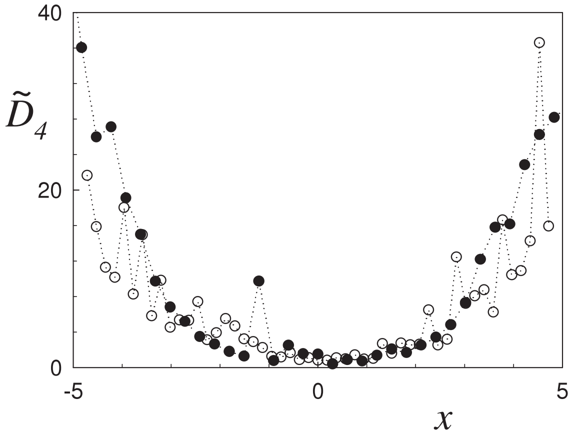

Figure 5. Coefficient $\tilde{D}_4$ obtained for the same data of figure 2 (filled symbols). Fourth finite-τ coefficient computed for an artificial time series generated with the coefficients D_1 and D_2 obtained by means of the exact parameters extracted from equations (6) and (7) (hollow symbols).

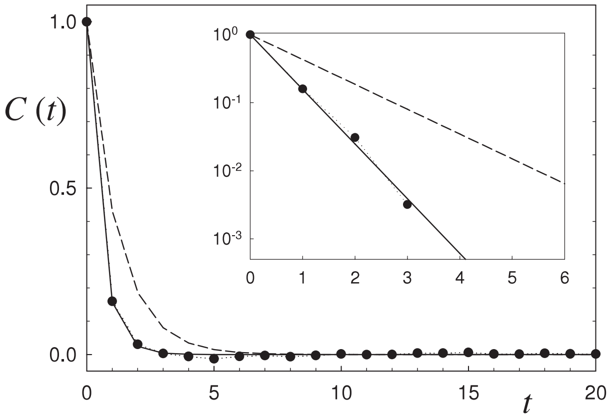

Figure 6. Linear auto-correlation $C(t)$ function versus time for the same data of figure 2 (filled circles). Theoretical functions $\exp(-a_1 t)$ (full line) and $\exp(-\tilde{a}_1 t)$ (dashed line). Inset: log–linear representation.

the empirical results. For instance, in figure 6, we observe an excellent agreement between the empirical linear auto-correlations and the theoretical prediction given by $\exp(-a_1 t)$. Conversely, the finite-τ parameter $\tilde{a}_1$ leads to overestimation of the linear correlation. From the above analysis, the linear–quadratic model constitutes a good description in this case and one can infer the actual parameters of the system from finite-τ measurements.

4. Concluding remarks

We have exploited the exact corrections for the linear–quadratic forms of first and second finite-time KM coefficients. Practical criteria arise that allow us to validate this model. The outcomes of our analysis go beyond the linear–quadratic paradigm. In particular, the results for the deterministic component are also valid for an arbitrary noisy component

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as soon as the drift is linear. That is, even in some cases where the Markov property is not strictly satisfied, for instance, if the noise is colored, the present strategy can still be used to disclose the deterministic component of the dynamics [17].

We investigated two real-world examples in which linear drift and quadratic diffusion coefficients are observed. However, in the former case, the linear–quadratic model fails. This shows that care must be taken when interpreting linear and quadratic forms arising from finite-time analysis, because they are not exclusive of the linear–quadratic model. Conversely, in the latter example, the linear–quadratic model is suitable, but the finite-time estimates significantly differ from the true values. In this case, low-order corrections are not enough and the exact corrections were successfully applied.

Our findings suggest that the analysis of observed linear and quadratic forms might be revised under the light of the present approach, both to check the model and to apply the appropriate corrections. We have also pointed out that those forms can emerge for arbitrary drift and diffusion coefficients when the independence limit is approached. All these warnings concern finite-time analysis of Markovian diffusion processes with generic forms of drift and diffusion coefficients (not necessarily polynomial) as well as in more general processes, even non-Markovian.

Acknowledgments

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