On the definition and handling of different drift and diffusion estimates

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Abstract. A previously devised approach for the reconstruction of Langevin processes from given data is revised with respect to disturbances stemming from finite sampling rates and the presence of external measurement noise. For these two cases and a combination of both three different estimates for the drift and diffusion functions are introduced, and an optimization procedure is presented that allows the reconstruction of the intrinsic functions from these estimates. Special attention is paid to the reconstruction of deterministic fixed points defining the characteristic behaviour of a process, and its robustness against the considered disturbing effects.

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1. Introduction

Complex dynamical systems appear in various scientific disciplines, and a suitable mathematical description is often of central interest. Revealing the process dynamics is realized by reconstructing the corresponding dynamic equations and finding a model for the dynamics of the studied systems. Prior to the reconstruction, the analysis is usually constrained to a special class of processes. A fundamental distinctive feature is, e.g. whether one applies a deterministic or a stochastic framework. Observed complex fluctuations can thus be traced back either to a chaotic behaviour or the effect of some dynamical noise. A more flexible approach is to combine both features and analyse a system in terms of general stochastic processes.

Here, we consider the class of Langevin processes, i.e. stochastic processes that are assumed to be Markovian and described in terms of drift and diffusion. A one-dimensional Langevin process is given by the stochastic first-order differential equation

\[
\dot{x}(t) = D^{(1)}(x) + \sqrt{D^{(2)}(x)} \Gamma(t),
\]

(also called the Langevin equation). Even though we restrict our discussion here to the one-dimensional case, it is straightforward to extend the argument to higher dimensional processes. The term \(D^{(1)}(x)\) is named the drift coefficient and reflects the deterministic part of the dynamics. The stochastic part is given by the Langevin force \(\Gamma(t)\), representing Gaussian white noise with \(\langle \Gamma(t) \rangle = 0\) and \(\langle \Gamma(t_1) \Gamma(t_2) \rangle = 2\delta(t_1 - t_2)\) (following the convention in [1]), and the square root of the diffusion coefficient \(D^{(2)}(x)\), fixing the amplitude of the stochastic fluctuations. Throughout the paper, we apply Itô’s interpretation of stochastic integrals.

Equation (1) is directly connected to the Fokker–Planck equation

\[
\frac{\partial}{\partial t} p(x, t) = \left[ -\frac{\partial}{\partial x} D^{(1)}(x) + \frac{1}{2} \frac{\partial^2}{\partial x^2} D^{(2)}(x) \right] p(x, t)
\]

describing the process in probability space.

In recent years, a method has been introduced to reconstruct the coefficients \(D^{(n)}(x)\) \((n = 1, 2)\) directly from a measured time series [2]–[5]. As initially proposed by Siegert et al, drift and diffusion coefficients can be derived according to

\[
D^{(n)}(x) = \frac{1}{n!} \lim_{\tau \to 0} \frac{1}{\tau} \langle M^{(n)}(x, \tau) \rangle,
\]

with the first \((n = 1)\) and second \((n = 2)\) conditional moment, respectively, given by

\[
M^{(n)}(x, \tau) := \langle [x(t + \tau) - x(t)]^n \rangle_{x(t) = x}.
\]

For an ideal time series, i.e. a time series \(x(t)\) that is generated by a process given by (1) and sampled over a sufficiently long time period and with a sufficiently high resolution, the process dynamics can be perfectly reconstructed by (3) and (4). For real data sets, however, the method of reconstruction must be revised with respect to several kinds of aspects—three of them are discussed in the following.

An observed time series \(x(t)\) is defined by a finite sampling rate. Thus, the continuous process given by (1) is reduced to a series of discrete points separated by the time increment \(\tau_0\).

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1 It is equally possible to reformulate the approach using other interpretations of stochastic integrals, for instance Stratonovich’s definition (cf [1]). In this definition, the drift coefficient is altered by an additional term, the spurious drift, and the reconstruction scheme is adapted correspondingly. But in total we do not expect to obtain fundamentally new insights.
corresponding to the inverse sampling rate, and information from smaller timescales is ignored (see figures 1(a) and (b)). Equation (1) is replaced by the discrete equation

$$x(t + \tau) = x(t) + \tau D^{(1)}(x) + \sqrt{\tau D^{(2)}(x)} \Gamma'(t),$$

where the $\Gamma'(t)$ correspond to independent Gaussian-distributed random numbers with zero mean and variance 2. Applying a conditional ensemble average and using the properties of $\Gamma'(t)$ specified above, we obtain as finite-$\tau$ approximations

$$M^{(1)}(x, \tau) \approx \tau D^{(1)}(x),$$

and

$$M^{(2)}(x, \tau) \approx 2\tau D^{(2)}(x) + \tau^2 (D^{(1)}(x))^2.$$  

That is $M^{(2)}(x, \tau)$ is modified by a correction term that is quadratic in $D^{(1)}(x)$ and $\tau$ and that vanishes in the limit $\tau \to 0$. Friedrich et al have shown in [6] that additional terms for $M^{(2)}(x, \tau)$
as well as for $M^{(1)}(x, \tau)$ are obtained when deriving the $\tau$-dependence of the conditional moments directly from the Fokker–Planck equation. For the approximations (6a) and (6b), however, a simplified transition probability is assumed (cf [7]). Ignoring any $O(\tau^2)$-corrections and using the simple relation $D^{(n)}(x) = M^{(n)}(x, \tau_0)/(n!\tau_0)$ for the analysis of non-ideal data, the empirical estimates may significantly differ from the intrinsic functions $D^{(n)}(x)$ ($n = 1, 2$) (cf [8]).

Similar deviations are observed when the time series $x(t)$ is superimposed by external measurement noise—see figure 1(c). The respective correction terms can be derived likewise, as presented in [9]. It is important to note that in both cases, for a not sufficiently small resolution as well as in the presence of external noise, the actual dynamics of the considered Langevin process is merely hidden but not destroyed. The challenge is to define corresponding estimates that are adjusted to the disturbance and to interpret the results in an appropriate way, or to introduce an appropriate optimization scheme that allows to reconstruct the intrinsic functions from the estimates.

The situation is a bit different, and this is the third aspect we address, if the requirement of the Markov property for the process given by $x(t)$ is not strictly fulfilled. Following [1], this is the case if the stochastic force $\Gamma(t)$ in (1) does not correspond to Gaussian-distributed and especially $\delta$-correlated white noise. For such non-Markovian processes, (3) and (4) can still be used to reconstruct the deterministic part of the process dynamics. Experimental evidence has been presented by Siefert et al [10] having reconstructed the drift coefficient $D^{(1)}(x)$ properly according to (3) for noise sources that are not Langevin forces and especially not $\delta$-correlated.

Allowing explicitly the non-Markovianity and non-Gaussianity of the noise source, the presented reconstruction scheme can be extended to a broader class of processes while its relevance is reduced to the deterministic part of the dynamics. A further extension, associated with a further reduction of significance, is achieved by considering not the entire deterministic dynamics of the process but just focusing on its characteristic or say global behaviour. For instance, it might be interesting to reconstruct only the deterministic fixed points $x_{FP}$ of an observed process. These are defined by

$$D^{(1)}(x_{FP}) \equiv 0. \tag{7}$$

The derivative of $D^{(1)}(x)$ in the neighbourhood of $x_{FP}$ determines the type of local stability. For a stable fixed point $(D^{(1)}(x))'|_{x=x_{FP}}$ is negative, for an unstable fixed point positive. A respective application is given in [11]. Here, the characteristic power curve of a wind turbine, i.e. the curve of steady states of power output for certain wind speeds, is determined by reconstructing the deterministic fixed points of the process binned according to the speed. It has been shown in [12] that the fixed points are more appropriate to characterize the power performance of the wind turbine system than maxima or mean values which are used for the standard procedure. The question arises how robust fixed points are against spoilings like the presence of external noise and finite sampling rates. An answer will be given at the end of this paper. Further applications are given in [13, 14], where the authors analysed traffic flows and the segregational dynamics in avalanches, respectively, with similar approaches.

This paper is arranged as follows. Following this introduction, we give an overview of the finite time and measurement noise corrections introduced in [7] and [9], respectively. In section 4, we compare both effects with each other, define distinctive features and introduce a scheme to combine them. Thereby, we develop three different estimates that are utilized for an optimized reconstruction of the intrinsic functions in section 5 and discussed with respect to
their significance, especially with regard to a proper reconstruction of fixed points, in section 6.
We conclude with section 7 which summarizes the main results.

2. Definition of drift and diffusion estimates adapted to finite sampling rates

As annotated in [7], the estimation of drift and diffusion coefficients for real data generally suffers from finite sampling rates, i.e. a finite time increment \( \tau_0 \). Friedrich et al introduced in [6] respective corrections by deriving exact expressions for the conditional moments up to a specified order of \( \tau \) from the Fokker–Planck equation. In the following, we summarize these considerations before interpreting and applying the results.

The conditional moments \( M^{(n)}(x, \tau) \) \((n = 1, 2)\), as defined in (4), are formulated according to

\[
\langle [x(t + \tau) - x(t)]^n \rangle |_{x(t) = x} = \int \, dx \, (x - x')^n \, p(x, t + \tau | x', t),
\]

in terms of the conditional probability density function (pdf) \( p(x, t + \tau | x', t) \). This conditional pdf is the solution of the Fokker–Planck equation

\[
\frac{\partial}{\partial t} p(x, t + \tau | x', t) = \hat{L} p(x, t + \tau | x', t)
\]

with the Fokker–Planck operator

\[
\hat{L} = -\frac{\partial}{\partial x} D^{(1)} + \frac{\partial^2}{\partial x^2} D^{(2)}.
\]

The formal solution of (9) reads

\[
p(x, t + \tau | x', t) = \exp[\hat{L} \tau] \delta(x - x').
\]

Expanding it in a stochastic Itô–Taylor series yields

\[
p(x, t + \tau | x', t) = \sum_{k=0}^\infty \frac{(\hat{L} \tau)^k}{k!} \delta(x - x')
\]

(cf [1]). By inserting (12) into (8), we obtain exact expressions for the conditional moments for arbitrary \( \tau \) or, restricting the expansion (12) to some finite order, the respective approximations. In accordance with [6], we find as second-order approximations

\[
M^{(1)}(x, \tau) = \tau D^{(1)} + \frac{\tau^2}{2} \left[ D^{(1)}(D^{(1)})' + D^{(2)}(D^{(1)})'' \right] + O(\tau^3)
\]

(13a)

\[
M^{(2)}(x, \tau) = 2\tau D^{(2)} + \tau^2 \left[ (D^{(1)})^2 + 2D^{(2)} (D^{(1)})' + D^{(1)}(D^{(2)})' + D^{(2)}(D^{(2)})'' \right] + O(\tau^3).
\]

(13b)

In comparison to (6a) and (6b), we thus obtain additional terms of order \( O(\tau^2) \).

Following [15], we introduce as first estimate, adapted to finite sampling rates,

\[
D^{(n)}_{\tau, \tau_0}(x, t_0) := \frac{M^{(n)}(x, \tau_0)}{n! \tau_0}.
\]

(14)
Inserting the expressions (13a) and (13b) with known functions $D^{(1)}(x)$ and $D^{(2)}(x)$ gives a theoretical estimate. An empirical estimate for a specific time series is, on the other hand, obtained with definition (4) according to

$$D_{E,\tau}^{(n)}(x, \tau_0) = \frac{1}{n!\tau_0}([x(t + \tau_0) - x(t)]^n)|_{x(t) = x}. \quad (15)$$

The connection between both theoretical and empirical estimates, is directly given by (8)–(12).

Turning to the theoretical case, we have analysed the deviations of the estimates $D_{E,\tau}^{(n)}(x, \tau_0)$ from the original functions for different simple examples. For an Ornstein–Uhlenbeck process (given by $D^{(1)}(x) = -\alpha x$ and $D^{(2)}(x) = \beta$ with $\alpha, \beta = \text{const}$), we obtain as theoretical estimates

$$D_{E,\tau}^{(1)}(x, \tau_0) = -\alpha x \left(1 - \frac{\alpha \tau_0}{2}\right) + O(\tau_0^2), \quad (16a)$$

$$D_{E,\tau}^{(2)}(x, \tau_0) = \beta \left(1 - \alpha \tau_0\right) + \frac{\tau_0 \alpha^2}{2} x^2 + O(\tau_0^2). \quad (16b)$$

The estimate $D_{E,\tau}^{(1)}(x, \tau_0)$ differs from the original function by a decreased slope, the estimate $D_{E,\tau}^{(2)}(x, \tau_0)$ is characterized by an additional quadratic term. For the application, this means that a quadratic diffusion coefficient must not indicate multiplicative noise but can be caused by a too low sampling rate. While the behaviour of $D^{(2)}(x)$ is thus significantly affected by the finiteness of $\tau$, the behaviour of $D^{(1)}(x)$ changes just quantitatively but not qualitatively. In particular, the fixed point of the process is not affected and can be reconstructed by the estimate correctly.

Next, we consider a process with additive noise ($D^{(2)} = b$) and cubic drift ($D^{(1)}(x) = -\alpha x^3$). Figure 2 shows the estimate $D_{E,\tau}^{(1)}(x, \tau_0)$ for two different values of $\tau_0$ (dashed and dotted lines, respectively). For both cases, the characteristic behaviour of $D^{(1)}$ is again reproduced correctly by the estimate (13a)—at least locally. Globally, $D_{E,\tau}^{(1)}(x, \tau_0)$ indicates additional fixed points, to the left and to the right of the original fixed point and with the inverse type of stability. These artefacts depend sensitively on changes of $\tau_0$, and they disappear when we consider higher order terms in (13a). Estimates for the drift coefficient according to (14) including additionally the third-order terms of the expansion (12) are shown in figure 2 as grey lines. The corresponding third-order corrections to (13a) are given in the appendix. This example emphasizes that it is of particular importance how many terms we consider for the expansion in (12).

To summarize the impact of finite-$\tau$ effects, figure 3 illustrates, exemplarily for an Ornstein–Uhlenbeck process, the deviations between the empirical values and the theoretical functions for $M^{(1)}(x, \tau)$ as well as the deviation between the introduced estimate and the intrinsic function for the drift coefficient. (For the illustration, we restrict our investigations to the analysis of the first conditional moment. An extension to $M^{(2)}(x, \tau)$ is straightforward.) The empirical values for $M^{(1)}(x, \tau)$ (given by the symbols) are characterized by a curvature that is defined by the higher order terms in $\tau$. Their agreement with the analytical second- and third-order approximations (dot-dashed and dotted lines) indicates up to which value of $\tau$ the respective approximation is reliable. Furthermore, the illustration shows the deviation between the estimate $D_{E,\tau}^{(1)}(x, \tau_0)$ and the intrinsic function $D^{(1)}(x)$ by comparing the linear relations $\tau D_{E,\tau_0}^{(1)}(x, \tau)$ and $\tau D^{(1)}(x)$. They only agree in the limit $\tau \to 0$, i.e. when the linear approximation $M^{(1)}(x, \tau) = \tau D^{(1)}(x)$ is exact, and the larger the value of $\tau$, the larger the deviation between estimate and intrinsic functions for $D^{(1)}(x)$ is.

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3. Definition of drift and diffusion estimates adapted to the presence of measurement noise

The second disturbance we discuss in this paper is the presence of external measurement noise. Siefert et al have already discussed in [16] how adding measurement noise to signals generated from a Langevin process leads to fundamental modifications of the data analysis and the reconstruction of the dynamics. They considered the special case of Gaussian-distributed noise, defined by $\sigma \zeta(t)$ with $\langle \zeta(t) \rangle = 0$ and $\langle \zeta(t_1) \zeta(t_2) \rangle = \delta(t_1 - t_2)$ and $\sigma$ as the amplitude of the noise. The presence of external measurement noise means that instead of $x(t)$ the time series $y(t) = x(t) + \sigma \zeta(t)$ is measured, i.e. the intrinsic process is superimposed by the external noise.

Adopting these considerations, Böttcher et al [9] proposed an advanced approach for the reconstruction of drift and diffusion coefficients based on the calculation of the conditional moments $M^{(n)}_\sigma(y, \tau)$—note that $M^{(n)}_\sigma$ is actually the same function as $M^{(n)}$ (see definition (4)) but for the time series $y(t)$ instead of $x(t)$. We use this new notation to distinguish the cases
Figure 3. Empirical values and theoretical functions for the first conditional moment of an Ornstein–Uhlenbeck process ($\alpha = 1$, $\beta = 1$), and the deviation between the estimate $D_{E,\tau}(x, \tau_0)$ and the intrinsic function $D^{(1)}(x)$. The empirical values for $M^{(1)}(x = -0.7, \tau)$ (according to (4)) are given by the symbols, the second- and third-order approximations are denoted by the dot-dashed and dotted lines, respectively. The solid line represents the linear approximation $\tau D^{(1)}(x)$, the dashed line the relation $\tau D^{(1)}_{E,\tau}(x, \tau_0 = 0.5)$ with the estimate according to (14). The grey circle indicates the value $M^{(1)}(x, \tau_0 = 0.5)$ used for the derivation of the estimate.

with and without external noise and to avoid confusion. Again, we summarize the corresponding procedure before we utilize it to define an appropriate estimate. Böttcher et al pointed out that the coefficients $D^{(n)}(x)$ are implicitly given by the conditional moments of the accessible data $y(t)$ according to

$$M^{(1)}(y, \tau) = \langle y(t + \tau) - y(t) \rangle \big|_{y(t)=y=x(t)+\sigma \zeta(t)} = \tau \int dx D^{(1)}(x) f(x|y) + \int dx (x - y) f(x|y) = m^{(1)}(y, \tau + \gamma_1(y))$$

(17a)

and

$$M^{(2)}(y, \tau) = \langle [y(t + \tau) - y(t)]^2 \rangle \big|_{y(t)=y=x(t)+\sigma \zeta(t)} = \tau \int dx \left[ 2(x - y)D^{(1)}(x) + 2D^{(2)}(x) \right] f(x|y) + \sigma^2 + \int dx (x - y)^2 f(x|y) = m^{(2)}(y, \tau) + \gamma_2(y),$$

(17b)

assuming afore that the approximation

$$M^{(n)}(x, \tau) \approx \tau n! D^{(n)}(x) + \mathcal{O}(\tau^2)$$

(18)
for $\tau \ll 1$ holds. The unknown probability density $f(x|y)$ is defined by

$$f(x|y) = \frac{f(y|x)p(x)}{\int dx f(y|x)p(x)},$$

(19)

where $f(y|x)$ is the distribution of the measurement noise, i.e. for Gaussian distributed noise

$$f(y|x) = \sqrt{\frac{1}{2\pi \sigma^2}} \exp \left[-\frac{(y-x)^2}{2\sigma^2}\right]$$

(20)

and $p(x)$ the distribution of the process $x(t)$, in the stationary case given by

$$p(x) = \frac{N}{D^{(2)}} \exp \left[\int_{-\infty}^{x} \frac{D^{(1)}(\tilde{x})}{D^{(2)}(\tilde{x})} dx\right]$$

(21)

with the normalization constant $N$ (cf [1]). Equations (17a) and (17b) indicate that the presence of measurement noise results in an offset $\gamma_0(y)$ for the conditional moments as function of $\tau$. In order to deal with the divergence of $M^{(a)}_\sigma(y, \tau)/\tau$ resulting from this offset, we suggest to define

$$D^{(n)}_{E,\sigma}(y) := \frac{m^{(n)}(y, \tau)}{n! \tau},$$

(22)

as second estimate for the drift and diffusion coefficients, respectively, adapted to the presence of external measurement noise. The theoretical estimate is hence determined by the first part in (17a) and (17b). An empirical estimate is calculated by applying a linear fit to $M^{(a)}_\sigma(y, \tau)$.

For a general process, (17a) and (17b) must be evaluated numerically. For an Ornstein–Uhlenbeck process as defined above, however, we can check the effect of the approximation (22) analytically. In [9], the terms $\gamma_0(y)$ and $m^{(n)}(y, \tau)$ were derived to

$$\gamma_1(y) = -\frac{\sigma^2}{\lambda^2} y, \quad \gamma_2(y) = \sigma^2 + \frac{\sigma^2 s^2}{\lambda^2} + \frac{\sigma^4}{\lambda^4} y^2$$

(23)

and

$$m^{(1)}(y, \tau) = \tau \left[-\alpha y - \alpha \gamma_1(y)\right],$$

$$m^{(2)}(y, \tau) = 2\tau (\beta - \alpha ([\gamma_2(y) - \sigma^2] + y\gamma_1(y)))$$

(24)

with $\lambda^2 := s^2 + \sigma^2$ and $s^2 = \beta/\alpha$ as the variance of the distribution $p(x)$. It follows that

$$D^{(1)}_{E,\sigma}(y) = -\alpha y \left(1 - \frac{\sigma^2}{\lambda^2}\right),$$

(25a)

$$D^{(2)}_{E,\sigma}(y) = \beta \left(1 - \frac{\sigma^2}{\lambda^2}\right) + \alpha \left(\frac{\sigma^2}{\lambda^2} - \frac{\sigma^4}{\lambda^4}\right) y^2.$$

(25b)

That is, in the presence of measurement noise, similar to the case of a finite sampling rate, the estimate for $D^{(1)}(x)$ differs from the original function quantitatively but not qualitatively. The absolute slope $\alpha$ is reduced by a factor depending on $\sigma$. The behaviour of $D^{(2)}_{E,\sigma}(y)$, on the other hand, is also qualitatively influenced by the external noise. The constant term $\beta$ is not only reduced by the same factor depending on $\sigma$ but additionally superimposed by a quadratic term.

For illustration, figure 4 compares the theoretical and empirical values for $M^{(1)}_\sigma(y, \tau)$ as well as the estimate $D^{(1)}_{E,\sigma}(y)$ and the undisturbed intrinsic drift function for an
Figure 4. Empirical values (symbols) and theoretical function (dotted line) for the first conditional moment $M_\sigma^{(1)}(y = -0.7, \tau)$ of an Ornstein–Uhlenbeck process ($\alpha = 1$, $\beta = 1$) that is superimposed by measurement noise ($\sigma = 0.5$). The solid line denotes the relation $\tau D^{(1)}(y)$ for the undisturbed case without external noise, the dashed line gives the relation $\tau D_{E,\sigma}^{(1)}(y)$ with the estimate according to equation (22).

We have analytically shown in the preceding two sections that for an Ornstein–Uhlenbeck process both a finite resolution defined by $\tau_0$ and the presence of external noise lead to very similar deviations of the introduced estimates from the original functions $D_{E}^{(n)}(x)$ ($n = 1, 2$). To illustrate this, figure 5 shows the empirical values as well as the theoretical functions for $D_{E}^{(n)}(x, \tau)$ and $D_{E,\sigma}^{(n)}(y)$ for an Ornstein–Uhlenbeck process ($\alpha = 1$, $\beta = 1$) that is sampled with $\tau_0 = 0.2$ for the first case and for the second superimposed by some external noise with $\sigma = 0.5$. Especially striking is the quadratic behaviour of the estimates for the diffusion coefficient.
Figure 5. Empirical and theoretical estimates $D_{E,\tau}^{(n)}$ and $D_{E,\sigma}^{(n)}$ ($n = 1, 2$) for an Ornstein–Uhlenbeck process ($\alpha = 1, \beta = 1$). The symbols represent the empirical results, the lines the theoretical functions—open symbols and dotted line for $\tau_0 = 0.2$ and $\sigma = 0$ (third-order corrections), full symbols and dashed line for $\tau_0 = 10^{-3}$ and $\sigma = 0.5$. The solid lines indicate the original functions $D^{(1)}(x)$ and $D^{(2)}(x)$.

In the case of a finite sampling rate $\tau_0$ this has already been detected in the approximation (6b) with the correction term $\tau^2(D^{(1)})^2$. An estimate that is adapted to this correction would reduce, though not eliminate the quadratic effect. This is different for the case of a nonzero $\sigma$, i.e. in the presence of measurement noise. Hence, it is essential to connect the results for the estimates with the observations for the conditional moments. Whereas a nonzero offset is an indicator for the presence of external noise, finite-$\tau$ effects are directly connected to a nonlinear curvature of $M^{(n)}(x, \tau)$ as function of $\tau$. Checking these two indicators gives information about which kind of disturbance is present and which definition of estimate has to be applied. Note that this is a central result for the application of the presented method of reconstruction.

To take a further step, we next consider a process that is affected by a finite sampling rate and external noise likewise. The considerations above suggest a certain hierarchy of both effects. The presence of external noise effectively changes the observable process, whereas the
value of $\tau_0$ just determines when and at which rate the process is observed. Consequently, we start with the considerations of section 3 and reformulate (17a) and (17b) as

$$M_\sigma^{(1)}(y, \tau) = \int dx M^{(1)}(x, \tau) f(x | y) + \int dx (x - y) f(x | y)$$

$$= m^{(1)}(y, \tau) + \gamma_1(y)$$  \hspace{1cm} (26a)

and

$$M_\sigma^{(2)}(y, \tau) = \int dx [2(x - y) M^{(1)}(x, \tau) + M^{(2)}(x, \tau)] f(x | y) + \sigma^2 + \int (x - y)^2 f(x | y)$$

$$= m^{(2)}(y, \tau) + \gamma_2(y),$$  \hspace{1cm} (26b)

expanding the moments $M^{(n)}(x, \tau)$ $(n = 1, 2)$ according to (8) and (12). Considering once again an Ornstein–Uhlenbeck process, the conditional moments for the undisturbed process with finite $\tau$ are given by

$$M^{(1)}(x, \tau) = -\tau a(\alpha, \tau) x,$$  \hspace{1cm} (27a)

$$M^{(2)}(x, \tau) = 2\tau [b(\alpha, \beta, \tau) + c(\alpha, \tau) x^2]$$  \hspace{1cm} (27b)

with appropriate definitions of the functions $a = a(\alpha, \tau)$, $b = b(\alpha, \beta, \tau)$ and $c = c(\alpha, \tau)$, dependent on how many terms we consider in (12). (The explicit functions for third-order approximations are given in the appendix.) Inserting (27a) and (27b) into (26a) and (26b), we obtain

$$m^{(1)}(y, \tau) = \tau [-a(\alpha, \tau) \left(1 - \frac{\sigma^2}{\lambda^2}\right) y],$$  \hspace{1cm} (28a)

$$m^{(2)}(y, \tau) = 2\tau \left\{b(\alpha, \beta, \tau) - a(\alpha, \tau) \left[\frac{\sigma^2 \lambda^2}{\lambda^2} + \left(\frac{\lambda^4 - \sigma^2}{\lambda^2}\right) y^2\right] + c(\alpha, \tau) \left[\frac{\sigma^2 \lambda^2}{\lambda^2} + \frac{s^4}{\lambda^4} y^2\right]\right\},$$  \hspace{1cm} (28b)

the terms for the offsets $\gamma_1(y)$ and $\gamma_2(y)$ remain unchanged (see (23)).

Figure 6 shows the empirical values $M_\sigma^{(1)}(y, \tau)$ for an Ornstein–Uhlenbeck process, similarly as in figure 4 but over a broader range of $\tau$, together with the theoretical approximation according to (28a) (third-order approximation for $M^{(1)}(x, \tau)$). Additionally, the linear relation $\tau D^{(1)}(y)$ including the intrinsic drift function and the relation $\tau D^{(1)}_{E, \tau}(y, \tau_0)$ are depicted where the estimate $D^{(n)}_{E, \tau}(y, \tau_0)$ $(n = 1, 2)$ is defined as follows.

Since we have to deal with a nonlinear behaviour due to a comparatively large $\tau_0$ and an (initially unknown) offset due to the measurement noise, simultaneously, neither the estimate defined by (14) nor that of (22) are practicable. Instead we suggest to define as a third estimate

$$D^{(n)}_{E, \tau}(y, \tau_0) := \frac{M^{(n)}_\sigma(y, 2\tau_0) - M^{(n)}_\sigma(y, \tau_0)}{n! \tau_0},$$  \hspace{1cm} (29)

where $\tau_0$ is the smallest available time increment or the sampling rate of the process, i.e. we simulate a linear fit to overcome the nonzero offset, but minimize the number of fitted points to reduce the impact of the nonlinear curvature.

We notice that $D^{(n)}_{E, \tau}(y, \tau_0)$ deviates considerably from the original function $D^{(n)}(x)$, especially for large values of $\tau_0$. Without measurement noise it converges to the intrinsic
Figure 6. Empirical values and theoretical functions for the first conditional moment of an Ornstein–Uhlenbeck process ($\alpha = 1$, $\beta = 1$) superimposed by external measurement noise ($\sigma = 0.5$), and the deviation between the estimate $D_{E,\tau\sigma}^{(1)}(y, \tau_0)$ and the intrinsic function $D^{(1)}(x)$. The empirical values for $M^{(1)}_\sigma(y = -0.6, \tau)$ are given by the symbols, the theoretical function is denoted by the dotted line (third-order approximation). The solid line represents the linear relation $\tau D^{(1)}(y)$, the dashed line the relation $\tau D_{E,\tau\sigma}^{(1)}(y, \tau_0 = 0.5)$ with the estimate according to equation (29). The grey circles indicate the values $M_{\sigma}^{(1)}(y, \tau_0 = 0.5)$ and $M_{\sigma}^{(1)}(y, \tau_0 = 1.0)$ used for the derivation of the estimate.

function for $\tau_0 \to 0$. For $\sigma \neq 0$, however, there is still in this limit an offset that corresponds to the deviation already shown in figure 4. The estimate $M_{\sigma}^{(1)}(y, \tau_0)/\tau_0$, analogously to (14), would actually provide results closer to $D^{(n)}(x)$ for certain values of $\tau_0$. The latter, however, diverges for small $\tau_0$ and is for this reason not suitable. Figure 7 gives an illustration of the discussed behaviour. Note that although the deviations between the estimates and the corresponding intrinsic function are quite large for most cases, the former can be utilized to extract the actual $D^{(n)}(x)$ with a good precision, as we show in the next section.

5. Reconstruction of the intrinsic drift and diffusion functions from the estimates through optimization

In this section, we present how the intrinsic functions $D^{(n)}(x)$ can be reconstructed from the estimates $D_{E,j}^{(n)}(j = \tau, \sigma, \tau\sigma)$. Following [9], where the disturbance by external noise has been considered (but not yet the case of low sampling rates), the basic idea is to minimize the sum of the squared deviations between the empirical estimates and the theoretical correspondents. The
**Figure 7.** Convergence behaviour of the estimates $D_{E,\tau}^{(1)}$ and $D_{E,\tau\sigma}^{(1)}$ for an Ornstein–Uhlenbeck process ($\alpha = 1$, $\beta = 1$) with and without measurement noise ($\sigma = 0.5$). The lines correspond to the theoretical estimates derived on the basis of the third-order approximations for the conditional moments.

A general procedure is as follows: for a given data set, the conditional moments are calculated for different values of $x$ or $y$, respectively, and plotted as function of the respective time increment $\tau$. An offset and/or a nonlinear curvature in these plots are indicators for certain disturbances. The according type of estimate adapted to the respective disturbance is selected, and the empirical values of the estimate are calculated directly from the data. Considering an appropriate parametrization $Q = \{q_i\}$ for the corresponding intrinsic functions $D_{E}^{(n)}(x)$, the theoretical estimates are calculated either analytically or numerically. Finally, the sum of the squared deviations between empirical and theoretical estimates is minimized by varying $Q$ and where necessary also the amplitude of the external noise assumed for the theoretical estimate. In contrast to [9], the single contributions to the total sum of deviations are additionally weighted by the variances $\sigma_{D_{E,\tau}^{(n)}}^2$ of the empirical estimates.

To demonstrate this procedure, we consider the example of a process defined by a linear drift ($D_{E,\tau}^{(1)}(x) = -ax$) and a quadratic diffusion coefficient ($D_{E,\tau\sigma}^{(2)}(x) = b + cx^2$). A process of this type is observed in various systems ranging from finance to turbulence or physiological time series (cf [17]–[19]). We have taken the values $a = 1$, $b = 0.1$ and $c = 0.5$ for the parameters and simulated time series consisting of $N = 5 \times 10^6$ data points in each case. For the first case, we took a sampling rate of $\tau_0 = 0.2$. A nonlinear curvature but zero offset in the plot of the conditional moments versus $\tau$ suggests to select the estimate $D_{E,\tau}^{(1)}(x)$ as defined in (14) and (15).

We calculated the empirical values for $D_{E,\tau}^{(n)}(x)$ and chose the parametrization $D_{E,\tau}^{(1)}(x) = -q_1x$ and $D_{E,\tau}^{(2)}(x) = q_2 + q_3x^2$, $Q = \{q_1, q_2, q_3\}$, to derive the theoretical estimates that will be denoted by $\hat{D}_{E,\tau}^{(n)}(x)$ for the following considerations. This notation indicates that the theoretical estimates are adapted to the empirical ones by variation of the set of parameters $Q$. Minimizing the sum
of weighted quadratic deviations, i.e.

$$\min_Q \left\{ \sum_i \left\{ \frac{1}{\sigma_{D_{E,r}^{(1)}}^2} [\hat{D}_{E,1}^{(1)}(x_i, \tau_0) - D_{E,1}^{(1)}(x_i, \tau_0)]^2 + \frac{1}{\sigma_{D_{E,r}^{(2)}}^2} [\hat{D}_{E,2}^{(2)}(x_i, \tau_0) - D_{E,2}^{(2)}(x_i, \tau_0)]^2 \right\} \right\},$$

(30)

we obtained the optimized reconstructed values \(q_1 = 1.0 (\pm 0.01), q_2 = 0.10 (\pm 0.01)\) and \(q_3 = 0.51 (\pm 0.01)\) that are in good agreement with the values of the original parameters \(a, b\) and \(c\).

For the second case, we took a sampling rate of \(\tau_0 = 10^{-3}\) and added measurement noise with an amplitude of \(\sigma = 0.25\) to the simulated time series. (This is the example that has already been considered in [9].) We used the parametrization given above and performed the optimization

$$\min_Q \sigma \left\{ \sum_{n=1,2} \sum_i \left\{ \frac{1}{\sigma^{(n)}_{D_{E,o}}} [\hat{D}_{E,o}^{(n)}(y_i) - D_{E,o}^{(n)}(y_i)]^2 + \frac{1}{\sigma_{\gamma_n}^2} [\hat{\gamma}_n(y_i) - \gamma_n(y_i)]^2 \right\} \right\},$$

(31)

by varying the parameters \(Q\) and \(\sigma\), where \(\sigma\) denotes the varied value for \(\sigma\). We obtained the results \(q_1 = 0.96 (\pm 0.01), q_2 = 0.10 (\pm 0.01), q_3 = 0.51 (\pm 0.01)\) and \(\sigma = 0.25 (\pm 0.01)\).

For the third and last cases, we took a sampling rate of \(\tau_0 = 0.2\) as in the first case but added measurement noise with an amplitude of \(\sigma = 0.25\) to the simulated time series. We calculated the empirical estimates as defined in (29) and compared them with the theoretical values derived according to

$$\hat{D}_{E,r,\sigma}^{(n)}(y, \tau_0) := \frac{m^{(n)}(y, 2\tau_0) - m^{(n)}(y, \tau_0)}{n! \tau_0}.$$  

(32)

The (extrapolated) offsets of the corresponding conditional moments are given by

$$\gamma_{n,E}(y, \tau_0) := 2 M_{\sigma}^{(n)}(y, \tau_0) - M_{\sigma}^{(n)}(y, 2\tau_0)$$

(33)

and

$$\hat{\gamma}_{n,E}(y, \tau_0) := 2 m^{(n)}(y, \tau_0) - m^{(n)}(y, 2\tau_0) + \hat{\gamma}_n$$

(34)

for the empirical and the theoretical cases, respectively. We performed the optimization task

$$\min_Q \sigma \left\{ \sum_{n=1,2} \sum_i \left\{ \frac{1}{\sigma^{(n)}_{D_{E,o}}} [\hat{D}_{E,o}^{(n)}(y_i, \tau_0) - D_{E,o}^{(n)}(y_i, \tau_0)]^2 + \frac{1}{\sigma_{\gamma_n}^2} [\hat{\gamma}_{n,E}(y_i, \tau_0) - \gamma_{n,E}(y_i, \tau_0)]^2 \right\} \right\},$$

(35)

by varying \(Q\) and \(\sigma\), and obtained as results \(q_1 = 0.98 (\pm 0.01), q_2 = 0.10 (\pm 0.01), q_3 = 0.47 (\pm 0.01)\) and \(\sigma = 0.25 (\pm 0.01)\). Figure 8 shows, exemplarily for this last case, the empirical values for the drift and diffusion estimates and the extrapolated offsets in comparison to the theoretical ones derived for the parameter sets \((Q, \sigma)\) and \((a, b, c, \sigma)\).

6. Handling the estimates and a note on the robustness of fixed points

For real data sets, an optimization procedure to reconstruct the intrinsic drift and diffusion functions from the disturbed estimates, as presented in the preceding section, is not always
Figure 8. Empirical (symbols) and theoretical (solid and dashed lines) estimates $D^{(1)}_{E, \tau_{\sigma}}(y)$ and extrapolated offsets $\gamma_{n,E}$ ($n = 1, 2$) for a process defined by the intrinsic functions $D^{(1)}(x) = -ax$ ($a = 1$) and $D^{(2)}(x) = b + cx^2$ ($b = 0.1$, $c = 0.5$) sampled with $\tau_0 = 0.2$ and spoilt by external measurement noise ($\sigma = 0.25$). Solid lines correspond to reconstructed and optimized set of parameters ($Q, \tilde{\sigma}$) and dashed lines to original parameters ($a, b, c, \sigma$).

realizable. By selecting a parametrization with a too high number of single parameters or considering too many orders of $\tau$ for the conditional moments, the procedure rapidly becomes very complex and expensive.

Furthermore, the procedure is strictly speaking not applicable to processes that are not of the Langevin type or Markov processes, respectively. As a rule, the data set at hand should be tested with regard to the Markov property prior to the analysis. Often one can find a typical length scale above which the process is Markovian even when this property is violated at lower scales (see e.g. [20]). Also promising is the fact, as shown in [21], that the presence of measurement noise itself spoils the Markov properties of an underlying Markov process. Hence,
limitations at small scales must not stem from the intrinsic properties of the underlying process
dynamics but might be the result of artificial noise sources that can be controlled much better
than the actual intrinsic dynamics.

As stated in the introduction, it might moreover even for non-Markovian processes make
sense to estimate at least the drift coefficient of such a process. Whereas the reconstruction of
the drift coefficient is not necessarily affected by a non-Markovianity of the process, we have
seen in sections 2–4 that it is significantly disturbed by finite-τ and noise effects. The question
arises whether the process dynamics can be reduced to a minimal characteristic behaviour of the
process that is not or is only weakly influenced by these effects. Reducing the drift dynamics to
some characteristic behaviour leads to the definition of its fixed points. Hence, the question is if
and how the fixed points of a certain process are affected by the discussed resolution and noise
effects. To give an answer, we assume again that we deal with a Langevin process.

From the analytical results obtained above we find that for an Ornstein–Uhlenbeck process
the position of the system’s fixed point is not at all influenced by the discussed effects. The
Ornstein–Uhlenbeck process is an absolutely symmetric process and the robustness of its
fixed point can just as well be deduced from simple symmetry arguments. For non-symmetric
processes, the case is more complicated. In figure 9, we show the theoretical estimates of
the drift coefficients for four exemplary processes in comparison to the intrinsic function
\( D^{(1)}(x) \) (each time as solid black line). The estimates for the finitely resolved process and
that superimposed by external noise—given by the dotted and dashed lines, respectively—have
been derived according to (14) and (22). For figure 9(a), we have considered a process with
linear drift and quadratic diffusion coefficients, both symmetric with respect to the fixed point.
The estimates seem to reproduce the fixed point robustly. (A very small deviation stemming
from the third-order finite-τ correction is not resolved by the figure.) Figure 9(b) also shows a
symmetric process but with multiple fixed points. The central fixed point is robust, whereas the
two outer points move with the estimates. It is clear that the central fixed point is determined
by a different symmetry from the two outer ones. While the shape of the drift coefficient is
compressed or stretched due to the finite-τ as well as measurement-noise effects which strongly
affect the outer fixed points, the central fixed point remains unchanged. The latter is seen here
as the centre of the symmetry. Figure 9(c) shows a process with asymmetric drift and constant
diffusion, and figure 9(d) one that is characterized by a shifted diffusion coefficient, otherwise
they are the same processes as in figure 9(a). In both cases, the estimates differ from the intrinsic
function for \( D^{(1)}(x) \) to a certain extent, and the fixed point is shifted due to the asymmetries.

In summary, we can conclude that symmetries in \( D^{(1)}(x) \) and \( D^{(2)}(x) \) are of extreme
importance for the robustness of fixed points in the presence of measurement noise and for
finitely resolved processes. Asymmetries in the estimates for drift and/or diffusion coefficients
are therefore to be utilized as indicators and warnings for potential shifting of the fixed points.
Finite-τ and measurement noise effects may lead to similar, i.e. equally directed, but also to
opposite deviations of the estimated fixed points compared to the intrinsic ones. Note that
the chosen values for \( \sigma \) correspond to very strong measurement noise. Similarly, the chosen
value for \( \tau_0 \) is quite large comparing it with the intrinsic time of the process that is given by
\( a^{-1} \) for a process with linear drift. The deviations between estimates and intrinsic functions
are accordingly large and should be regarded as upper limits rather than as typical results.
Nevertheless, the presented results show that even for these cases the structure of the considered
process, i.e. its approximate functional behaviour, could be unveiled by the estimates. A refined
approach is to relate the amplitude of the external noise as well as the resolution of the sampled
Figure 9. Theoretical drift estimates for four exemplary processes. (a) $D^{(1)}(x) = -ax$ and $D^{(2)}(x) = b + cx^2$ ($a = 1$, $b = 1$, $c = 0.5$), (b) $D^{(1)}(x) = ax - bx^3$ and $D^{(2)}(x) = c$ ($a = 1$, $b = 0.5$, $c = 1$), (c) $D^{(1)}(x) = -\exp(x) + 1$ and $D^{(2)}(x) = b + cx^2$ ($a = 1$, $b = 1$, $c = 0.5$), (d) $D^{(1)}(x) = -ax$ and $D^{(2)}(x) = b + c(x + d)^2$ ($a = 1$, $b = 1$, $c = 0.5$, $d = 2$)—each time with $\tau_0 = 0.2$, $\sigma = 0$ (dotted) and $\tau_0 \ll 1$, $\sigma = 1$ (dashed).

7. Conclusions

We have investigated how two different aspects influence the reconstruction of Langevin processes—a finite sampling rate and the presence of external measurement noise. For both time series with the nonlinearities of the intrinsic drift and diffusion functions. Since the fixed-point analysis is a local linear method, it is affected if and only if the disturbance brings the dynamics out of the linear vicinity of the fixed point.
disturbances we identified indicators, and introduced corresponding estimates for the drift and
diffusion functions defining the process. The different estimates essentially differ in how the
limit \( \tau \to 0 \) for the reconstruction is realized (cf (3)). Each kind of disturbance complicates
this limit in a specific way and the proposed estimates are adapted to the particular difficulty.
The significant contribution of this paper is that the two disturbances are not only discussed
separately, as in [6, 7, 9], but also combined. This allows for a more advanced application
of the method of reconstruction to real data. Note that our method also covers the case of
strong noise.

We have presented two possibilities of application—one is to reconstruct the intrinsic
drift and diffusion functions from the estimates utilizing an optimization scheme, and the
other is to reduce the reconstruction of the process dynamics to the estimation of its fixed
points. The proposed optimized reconstruction can be seen as an alternative to the iterative
procedure introduced in [22] with the advantage that it can be applied to processes suffering
from a finite sampling rate and the spoiling by external noise likewise. For the reconstruction of
the fixed points we have worked out the relevance of the symmetries of the underlying dynamic
equations. For asymmetric processes we showed that the derived estimates indicate fixed points
that are shifted in comparison to the intrinsic functions due to a finite sampling rate and/or the
presence of external measurement noise. Thus, we obtained an indicator for the robustness and
the quality of estimated fixed points and at the same time defined a frame for the application of
a reliable fixed-point method. Likewise, the disturbances are to be related to the nonlinearities
of the intrinsic functions. With this information, that is just obtained from the proposed method
of data analysis, a model for the considered system can be put up and fine-tuned optimizing the
estimates by iterative steps.

Appendix. Derivation of third-order terms

As third-order approximations for the conditional moments we find

\[
M^{(1)}(x, \tau) = \tau D^{(1)} + \frac{\tau^2}{2} \left[ D^{(1)}(D^{(1)})' + D^{(2)}(D^{(1)})'' \right] + \frac{\tau^3}{6} \left[ D^{(1)}(D^{(1)})'(D^{(1)})' + D^{(1)} D^{(1)}(D^{(1)})'' \\
+ 3D^{(2)}(D^{(1)})'(D^{(2)})'' + 2D^{(1)} D^{(2)}(D^{(1)})'' + D^{(1)}(D^{(2)})'' + D^{(2)}(D^{(1)})''(D^{(2)})'' \\
+ 2D^{(2)}(D^{(2)})'(D^{(1)})'' + D^{(2)} D^{(2)}(D^{(1)})'' \right] + O(\tau^4)
\]

(A.1)

and similarly for the second conditional moment

\[
M^{(2)}(x, \tau) = 2\tau D^{(2)} + \tau^2 \left[ (D^{(1)})^2 + 2D^{(2)}(D^{(1)})' + D^{(1)}(D^{(2)})'' + 2D^{(2)}(D^{(2)})'' \right] \\
+ \frac{\tau^3}{3} \left[ 3D^{(1)}(D^{(1)})' + 4D^{(1)}(D^{(1)})' + 7D^{(1)} D^{(2)}(D^{(1)})'' + 3D^{(1)}(D^{(1)})' (D^{(2)})'' \\
+ 4D^{(2)}(D^{(1)})'' + 7D^{(2)}(D^{(2)})'(D^{(2)})'' + 4D^{(2)}(D^{(1)})'(D^{(2)})'' + D^{(1)} D^{(1)}(D^{(2)})'' \\
+ 2D^{(1)} D^{(2)}(D^{(2)})'' + D^{(1)}(D^{(2)})'' + D^{(2)} D^{(2)}(D^{(2)})'' + 2D^{(2)}(D^{(2)})'' \right] + O(\tau^4).
\]

(A.2)

For an Ornstein–Uhlenbeck process \((D^{(1)}(x) = -ax \text{ and } D^{(2)}(x) = \beta)\) this gives

\[
M^{(1)}(x, \tau) = -\tau ax + \frac{\tau^2 a^2 x}{2} - \frac{\tau^3 a^3 x}{6} + O(\tau^4),
\]

(A.3)
\[ M^{(2)}(x, \tau) = 2\beta \tau + \tau^2 (2\alpha^2 x^2 - 2\alpha \beta) + \frac{\tau^3}{3} (-3\alpha^3 x^2 + 4\alpha^2 \beta) + O(\tau^4). \] (A.4)

Hence, the functions \( a = a(\alpha, \tau), b = b(\alpha, \beta, \tau) \) and \( c = c(\alpha, \tau) \), introduced in section 4, are given by

\[ a(\alpha, \tau) = \alpha - \frac{\tau \alpha^2}{2} + \frac{\tau^2 \alpha^3}{6}, \] (A.5)

\[ b(\alpha, \beta, \tau) = \beta - \tau \alpha \beta + \frac{2\tau^2}{3} \alpha^2 \beta \] (A.6)

and

\[ c(\alpha, \tau) = \frac{\tau}{2} \alpha^2 - \frac{\tau^2}{2} \alpha^3. \] (A.7)

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