ESTIMATION OF MEASUREMENT NOISE AND DYNAMICAL PARAMETERS FROM TIME SERIES DATA

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Abstract

One of the major challenges in the field of nonlinear time series analysis is the development of suitable tools dealing with data of complex systems generated by stochastic dynamical systems.

The main purpose of the present article is to describe a method which allows one to disentangle trends and fluctuations for the class of systems whose time evolution can be described by Langevin equations. The proposed method bypasses restrictions in the evaluation of drift and diffusion coefficients arising for data sets generated at low sampling rates. It is based on an iterative refinement of the estimation of drift and diffusion terms based on an optimization of Kullback entropy measuring the distance between experimentally and estimated probability distributions. Additionally, we address the problem how to handle data sets generated by Langevin equations, which additionally are contaminated by external noise.

Key words

Stochastic time series analysis, Langevin equation, Measurement noise

1 Introduction

Complex behavior in systems far from equilibrium can quite often be traced back to rather simple laws due to the existence of processes of selforganization (Haken, 2004). Since complex systems are composed of a huge number of subsystems, however, fluctuations stemming from the microscopic degrees of freedom play an important role introducing a temporal variation on a fast time scale which usually can be treated as fluctuations. A consequence of this rather general scheme is the existence of evolution equations of a set of macroscopic order parameters $\mathbf{q}(t)$ which are governed by nonlinear Langevin equations (Risken, 1989), (Gardiner, 2004):

$$\dot{q}_i = D_i^{(1)}(\mathbf{q}) + \sum_l g_{il}(\mathbf{q})\Gamma_l(t) \quad (1)$$

where $\mathbf{q}(t)$ denotes the n-dimensional state vector, $\boldsymbol{D}^{(1)}(\mathbf{q})$ is the drift vector and the matrix $g(\mathbf{q})$ is related to the diffusion matrix according to

$$\left(D_{ij}^{(2)}(\mathbf{q})\right)_{ij} = \sum_k g_{ik}(\mathbf{q})g_{jk}(\mathbf{q}) \quad . \quad (2)$$

$\boldsymbol{\Gamma}(t)$ are fluctuating forces with Gaussian statistics delta-correlated in time:

$$< \Gamma_l(t) > = 0 \quad , \quad (3a)$$

$$< \Gamma_l(t)\Gamma_k(t') > = 2\delta_{lk}\delta(t-t') \quad . \quad (3b)$$

Here and in the following we adopt Itô's interpretation of stochastic integrals (Risken, 1989), (Gardiner, 2004).

Analyzing complex systems, which can be described by stochastic equations of the form (1), therefore, amounts to assess the underlying Langevin equations or the corresponding Fokker-Planck equations from a treatment of experimentally determined time series (Haken, 2000). Recently, a method (Siegert *et al.*, 1998), (Friedrich *et al.*, 2000*b*) has been suggested, which determines drift and diffusion coefficients from the first and second conditional moments of the process:

$$\boldsymbol{D}^{(1)}(\mathbf{q}) = \lim_{\tau\to 0}\frac{1}{\tau} < \mathbf{q}(t+\tau) - \mathbf{q}(t)|\mathbf{q}(t) = \mathbf{q} > \quad (4a)$$

$$D_{ij}^{(2)}(\mathbf{q}) = \lim_{\tau\to 0}\frac{1}{2\tau} < [\mathbf{q}(t+\tau) - \mathbf{q}(t)]_i [\mathbf{q}(t+\tau) - \mathbf{q}(t)]_j|\mathbf{q}(t) = \mathbf{q} > \quad (4b)$$

This method has been successfully applied to various problems in the field of complex systems like the analysis of noisy electrical circuits (Friedrich *et al.*, 2000*b*), stochastic dynamics of metal cutting (Gradisek *et al.*, 2002), systems with feedback delay (Frank *et al.*, 2004), meteorological processes like wind-driven Southern Ocean variability (Sura and Gille, 2003) and traffic flow data (Kriso *et al.*, 2002). Furthermore it has been applied to problems like turbulent flows (Friedrich and Peinke, 1997), (Renner *et al.*, 2001), passive scalar advection (Tutkun and Mydlarski, 2004), financial time series (Friedrich *et al.*, 2000*a*), analysis of rough surfaces (Jafari *et al.*, 2003), (Wächter *et al.*, 2003), which can be characterized as a markovian stochastic process with respect to a scale variable.

The method is based on the evaluation of the time limits of the first and second conditional moments eq. (4). From these expressions it becomes evident that the sampling rate in the experiments has to be sufficiently high in order to allow for a reliable evaluation of the limit $\tau \to 0$. Possible problems in estimating drift and diffusion coefficients related with low sampling frequencies have been addressed by Sura (Sura and Barsugli, 2002), Ragwitz and Kantz (M. Ragwitz, 2001), Friedrich et al. (Friedrich *et al.*, 2002), and Ragwitz and Kantz (Ragwitz and Kantz, 2002).

If the underlying stochastic process is markovian the limits (4) yield the exact dynamical parameters of the Langevin equation. However, in some cases, the estimation of the limiting expressions may become difficult. Basically, there are three facts which render the estimates problematic. The first case is the presence of uncorrelated noise sources, so-called measurement noise (Siefert *et al.*, 2003). The second case appears if the sampling rate is not high enough for a reliable extrapolation to $\tau \equiv 0$. The third case arises if the process is nonmarkovian below a certain time scale.

The aims of this work therefore are twofold:

In section 2 a general method is proposed that overcomes problems arising through the time limit $\tau \to 0$.

In section 3 we discuss how to deal with time series contaminated by measurement noise. A general expression is devised to assess the strength of the external noise for the case of uncorrelated external fluctuations. Given a parametric model for the internal dynamics one is able to determine the model parameters and the strength of the noise source. In this way dynamical and external noise sources can be separated.

Time series of stationary stochastic processes usually can be assumed to be ergodic. For this reason probability density functions (pdf's) can be extracted from the data by averaging with respect to time. We adopt the following notation. Variables measured at time $t+\tau$ are denoted with a prime, q'.

2 An iterative procedure for the estimation of drift and diffusion terms

In this section we describe an iterative procedure for the extraction of drift and diffusion terms of data sets generated by Langevin equations. This procedure has been devised in order to overcome the difficulties arising in the evaluation of the limits (4) and is applicable to data sets sampled at low sampling rates.

A first estimate of drift and diffusion coefficients apparently is delivered by the expressions (4) evaluated for the smallest possible values of τ. The obtained functions can now be embedded into a family of functions $\boldsymbol{D}^{(1)}(\mathbf{q},\boldsymbol{\sigma})$, $D^{(2)}(\mathbf{q},\boldsymbol{\sigma})$ parameterized by a set of free parameters $\boldsymbol{\sigma}$. These parameters can be e.g. the coefficients of a Taylor series for $\boldsymbol{D}^{(\mathbf{1})}(\mathbf{q},\boldsymbol{\sigma})$ and $D^{(2)}(\mathbf{q},\boldsymbol{\sigma})$. The decisive step consists now in optimizing the free parameters $\boldsymbol{\sigma}$, where a first estimate already is available.

Optimization of the free parameters can be achieved on the basis of a comparison of the conditional probability distribution $p_\tau(\mathbf{q}'|\mathbf{q};\boldsymbol{\sigma})$ and the one obtained from experiment. The pdf for the parameter set $\boldsymbol{\sigma}$ can be determined either by a simulation of the Langevin equations or by a numerical solution of the corresponding Fokker-Planck equation. In each case, one can determine the two point pdf

$$P_\tau(\mathbf{q}',\mathbf{q};\boldsymbol{\sigma}) = p_\tau(\mathbf{q}'|\mathbf{q};\boldsymbol{\sigma})P(\mathbf{q}) \quad . \tag{5}$$

Here, we want to emphasize that the pdf can be estimated for various finite values of the time increment τ. The obtained two time pdf can now be compared with the experimental one P_τ^{exp}. A suitable measure for the distance between two pdf's is the Kullback-Leibler information (Haken, 2000) defined according to

$$K(\boldsymbol{\sigma}) = \iint d\mathbf{q}' d\mathbf{q}\, P_\tau^{exp}(\mathbf{q}',\mathbf{q}) \ln \frac{P_\tau^{exp}(\mathbf{q}',\mathbf{q})}{P_\tau(\mathbf{q}',\mathbf{q};\boldsymbol{\sigma})} \, . \tag{6}$$

The Kullback entropy is a function of the parameters $\boldsymbol{\sigma}$ which parameterize the drift and diffusion terms of the stochastic process. The process corresponding to the minimizing parameter set yields the best approximation with respect to this measure. The problem of identifying a stochastic process is then equivalent to determining a minimum of the Kullback information. In practice the minimum can be determined by gradient or genetic algorithms (Weinstein *et al.*, 1990) and solved by standard methods. In the following we shall consider cases, where it is possible to obtain a parametrization of the stochastic processes by only few parameters $\boldsymbol{\sigma}$ such that the Kullback-Leibler measure can be investigated graphically. This can be done for one dimensional Langevin equations and for the class of potential systems. In both cases, the analytical expressions for the stationary probability functions are known in terms of drift and diffusion functions. This knowledge can be exploited for data analysis.

2.1 One dimensional systems

The case of one-dimensional systems allows for the following treatment due to the fact that the stationary pdf, which is assumed to exist, can be determined analytically:

$$P(q) = \frac{N}{D^{(2)}(q)} e^{\int^{q} d\tilde{q} \frac{D^{(1)}(\tilde{q})}{D^{(2)}(\tilde{q})}} \tag{7}$$

As a consequence, we have the relationship

$$D^{(1)}(q) = D^{(2)}(q) \frac{d}{dq} \ln P(q) + \frac{d}{dq} D^{(2)}(q) \quad . \tag{8}$$

Since $P(q)$ can be determined from the time series an estimate in terms of a parametrized ansatz for the diffusion term suffices. In fact, one may use $D^{(2)}(q) = Q + aq^2 + bq^4 + \dots$, which helps by lowering the number of parameters $\boldsymbol{\sigma}$ to be estimated by the above procedure of minimization the Kullback-Leibler information. The drift then follows as indicated above. The analysis of an one-dimensional stochastic time series with multiplicative noise term is discussed in (Kleinhans *et al.*, 2005).

2.2 Application to potential systems

Let us now consider the so-called class of potential systems for which the drift vector $\boldsymbol{D}^{(1)}(\mathbf{q})$ is obtained from a potential $V(\mathbf{q})$ and $g_{ik} = \sqrt{Q}\delta_{ik}$. The central point of our analysis is the following exact expression for the stationary pdf

$$P(\mathbf{q}) = N e^{-V(\mathbf{q})/Q} \quad . \tag{9}$$

This relation yields the drift potential up to the noise strength Q from the stationary pdf,

$$V(\mathbf{q}) = -Q \ln \left[P(\mathbf{q}) \right] \quad . \tag{10}$$

Since the stationary pdf can be estimated from experimental data we can parameterize the class of stochastic processes by the single variable Q. Thus the drift function can be considered to be fixed except for the value Q:

$$\boldsymbol{D}^{(1)}(\mathbf{q}) = Q \nabla \ln P(\mathbf{q}) \tag{11}$$

Let us consider the following example in more detail. We use synthetic data obtained by numerical integration of the corresponding Langevin equation (Risken, 1989). In the iteration procedure the two point pdf's have to be calculated. We again use the numerical simulation of the Langevin equation as the most efficient way to generate the pdf's.

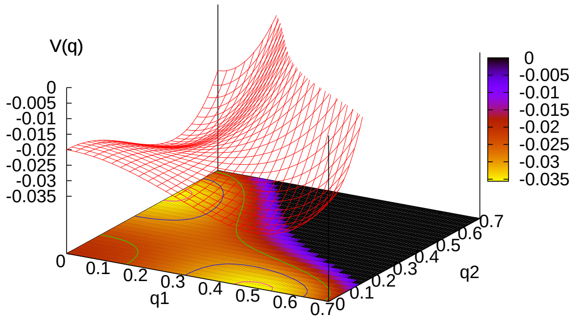

Figure 1. The potential $V(\mathbf{q})$ (eq. (13)) and corresponding contour plot for $B = 4$ and $\epsilon = 0.25$. The potential possesses minima at $(q_1 = \sqrt{\epsilon}, q_2 = 0)$, $(q_1 = 0, q_2 = \sqrt{\epsilon})$, corresponding to stable fixed points as well as the local maximum in the origin and a saddle point at $(q_1 = \sqrt{\epsilon/(1+B)}, q_2 = \sqrt{\epsilon/(1+B)})$.

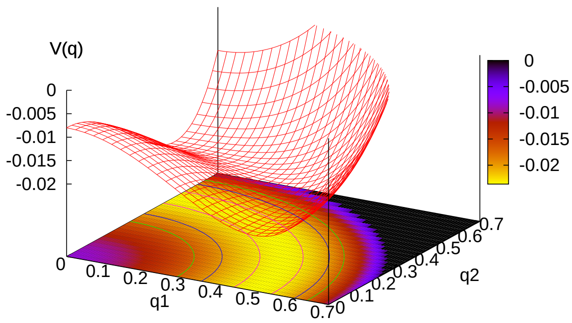

Figure 2. Detail of the model drift potential (eq. (13)) for $B = 1$, $\epsilon = 0.25$. It is the so-called wine-bottle potential with a degenerated concentric minimum with radius $\sqrt{\epsilon}$.

The two-dimensional system

$$D_1^{(1)}(\mathbf{q}) = \epsilon q_1 - q_1 \left(q_1^2 + B q_2^2 \right) \tag{12a}$$

$$D_2^{(1)}(\mathbf{q}) = \epsilon q_2 - q_2 \left(B q_1^2 + q_2^2 \right) \tag{12b}$$

with $\epsilon = 0.25$ is considered. It plays an important role in the theory of self-organization of complex systems (Haken, 1991). The drift vector field can be derived from the potential

$$V(\mathbf{q}) = -\frac{\epsilon}{2}\mathbf{q}^2 + \frac{1}{4}\mathbf{q}^4 + \frac{B-1}{2} q_1^2 q_2^2 \quad . \tag{13}$$

The potential is symmetric to the origin. Its shape depends on the parameter B as can be seen from fig. 1-3. The minima of the potential are stable, the saddle

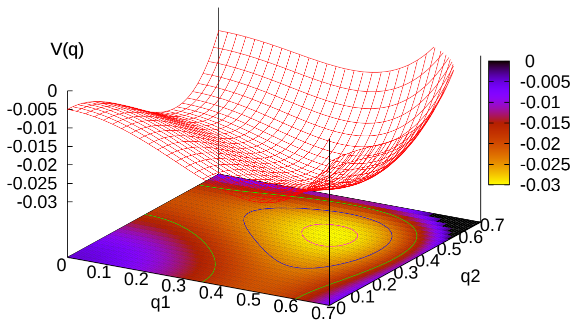

Figure 3. Detail of the model drift potential (eq. (13)) for B=0.25. The minimum on the bisection line can clearly be identified. The former minima have turned to saddle points, the maximum is still present.

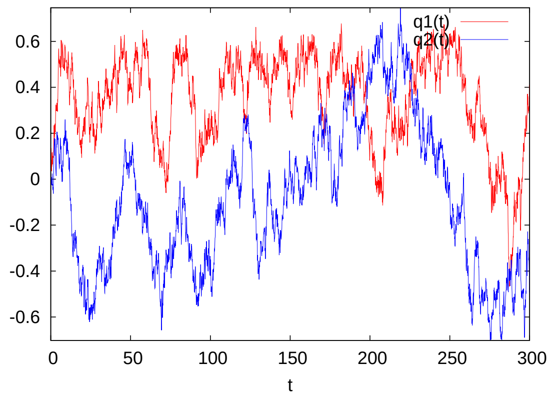

Figure 4. Detail of two-dimensional synthetic time series I.

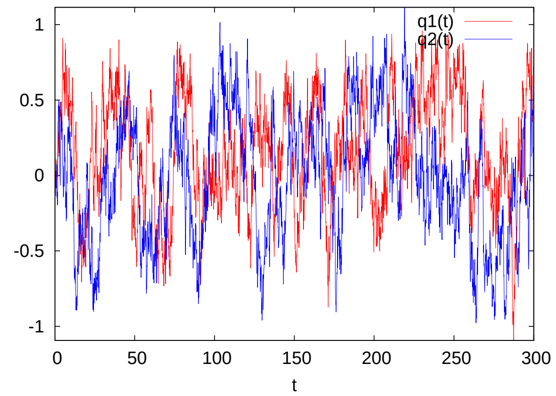

Figure 5. Detail of two-dimensional synthetic time series II.

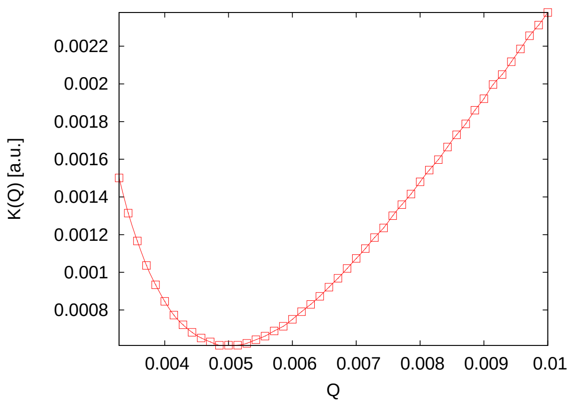

Figure 6. The Kullback distance K(Q) as a function of the noise strength Q (time series I). A minimum is clearly visible at the value Q=0.005.

points and maxima unstable fixed points of the dynamics. For $B > 1$ there are four minima on the q_1 and q_2 axes at $|\mathbf{q}| = \sqrt{\epsilon}$. The depth of this minima decreases with B. For $B \equiv 1$ it degenerates into the so-called *wine-bottle potential*, the rotationally symmetric equivalent of the double well potential with minima at $\pm\sqrt{\epsilon}$. For $B < 1$ the fixed point on the axis turn into saddle points and stable fixed points exist on the bisecting lines of the axes.

Synthetic data has been generated using the time increment $\tau = 0.1$. The time increment for numerical integration of the Langevin equation was chosen to $\tau = 10^{-4}$. The simulated time series consists of $5 \cdot 10^6$ data points. Two following parameter sets were used: Serie I with $Q = 0.005$ and $B = 0.96$ which is very closed to the concentric case of the potential. A part of the time series is exhibited in fig. 4. For series II we choose $Q = 0.05$ and $B = 2.0$ corresponding to a different system state. Figure 5 shows a part of the time series.

The drift $\boldsymbol{D}^{(1)}(\mathbf{q})$ can be evaluated from (11). The noise strength Q in this case is the only free parameter left. Since (11) yields a stationary distribution of the simulated process that equals the experimental one the Kullback distance (6) simplifies to

$$K(Q) = \iint d\mathbf{q}' d\mathbf{q}\, P_\tau^{exp}(\mathbf{q}', \mathbf{q}) \ln \frac{p_\tau^{exp}(\mathbf{q}'|\mathbf{q})}{p_\tau(\mathbf{q}'|\mathbf{q}; Q)} \; . \tag{14}$$

For evaluation of the joint pdf from data state space has to be divided in bins. We used 100×100 equidistant bins for the stationary pdf. The conditional pdf locally can be retrieved from the data for any $\mathbf{q}$ with high accuracy.

After evaluating the Kullback measure for various values of Q this value has to be optimized. The optimal value is determined by the minimum of the Kullback distance. As outlined above there are some efficient ways to determine the minimum. However, for our examples the minimum can easily be found graphically. Since for low values of Q p_τ gets localized at the minima of the potential the distance $K(Q)$ diverges for $p_\tau/p_\tau^{exp} \equiv 0$ for $Q \to 0$.

Figures 6 and 7 show the Kullback distance $K(Q)$ as

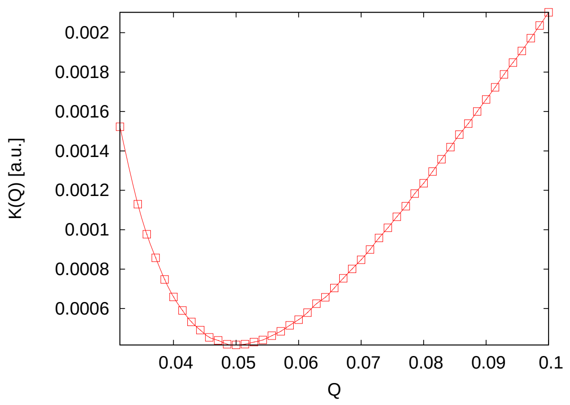

Figure 7. The Kullback distance K(Q) as a function of the noise strenght Q (time series II). The minimum is found at Q=0.05.

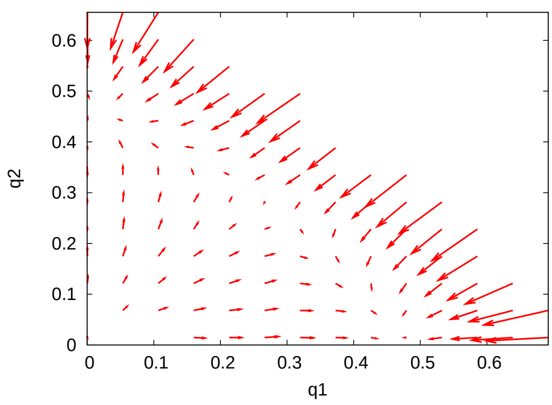

Figure 9. Time series II: Drift vector field extracted from data using the optimal value of Q. Unstable fixpoints in the center and on the bisection line as well as the attractive fixpoints are clearly visible.

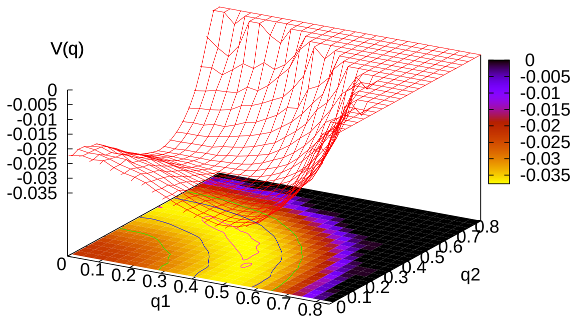

Figure 8. Drift potential reconstructured from time series I for optimal Q.

a function of the noise strength Q for the time series I and II. In both cases the minima are well-defined. The corresponding values of Q agree with the ones used for simulation. For these parameters the drift vector field and the corresponding potential can be recalculated from the stationary distribution using (10) and (11). The results are exhibited for the potential of series I in fig. 8 and for the drift vector field of dataset II in fig. 9.

3 Data contaminated by external noise

We consider a one-dimensional stationary stochastic dynamical process $q(t)$ that is superposed by measurement noise $\zeta(t)$:

$$y(t) = q(t) + \zeta(t) \quad . \tag{15}$$

While the dynamics of q is assumed to be governed by a Langevin equation (1) the external noise is uncorrelated and does not influence the internal dynamics of q.

3.1 Transition Probabilities

For the different processes the conditional transition pdf's $f\,(y|q)$ and

$$p_\tau(q'|q) = \frac{\langle \delta(q(t+\tau) - q')\delta(q(t) - q)\rangle}{\langle \delta(q(t) - q)\rangle} \quad . \tag{16}$$

can be defined. These pdf's enter into the expressions for the transition probability $g_\tau(y'|y)$ of the measured data y:

$$\begin{aligned} g_\tau(y'|y) &= \iint dq dq' \tilde{g}_\tau(y', q', q|y) \\ &= \iint dq dq' f(y'|q') p_\tau(q'|q) \tilde{f}(q|y) \end{aligned} \tag{17}$$

The conditional pdf's allows for specification of the conditional moments of the processes $y(t)$ and $q(t)$:

$$\begin{aligned} M_f^{(n)}(q) &= \langle [y(t) - q(t)]^n \rangle|_{q(t)=q} \\ &= \int dy [y - q]^n f\,(y|q) \end{aligned} \tag{18}$$

$$\begin{aligned} M_{p_\tau}^{(n)}(q) &= \langle [q(t+\tau) - q(t)]^n \rangle|_{q(t)=q} \\ &= \int dq' [q' - q]^n p_\tau\,(q'|q) \end{aligned} \tag{19}$$

$$\begin{aligned} M_{g_\tau}^{(n)}(q) &= \langle [y(t+\tau) - y(t)]^n \rangle|_{y(t)=y} \\ &= \int dy' [y' - y]^n g_\tau\,(y'|y) \end{aligned} \tag{20}$$

For small τ the moments of q (19) can be approximated by an Itô taylor expansion. Complying with (4) the lowest order expansion coefficients are the dynamical parameters $D^{(1)}$ and $D^{(2)}$:

$$M_{p_\tau}^{(1)}(q) = \tau D^{(1)}(q) + O(\tau^2) \tag{21}$$

$$M_{p_\tau}^{(2)}(q) = \tau D^{(2)}(q) + O(\tau^2) \tag{22}$$

For the sake of simplicity we assume the measurement noise to be gaussian with variance σ, which actually should be a realistic assumption. The conditional pdf reads

$$f(y|q) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(q-y)^2}{2\sigma^2}\right) \quad . \tag{23}$$

The first moment $M_f^{(1)}$ vanishes, the second $M_f^{(2)}$ is known to be σ^2.

Finally we will need the inverse pdf $\tilde{f}(q|y)$. Using bayesian statistics this can be calculated from

$$\tilde{f}(q|y) = \frac{f(y|q)P(q)}{F(y)} = \frac{f(y|q)P(q)}{\int dq f(y|q)P(q)} \quad . \tag{24}$$

3.2 First moment $M_{g_\tau}^{(1)}$

For the drift estimate from (4) for stochastic Langevin processes the first moment $M_{g_\tau}^{(1)}$ of the data has to be evaluated. For noisy data the first moments can be used as well. Taking advantage of the vanishing first moment of f this reads:

$$\begin{aligned} M_{g_\tau}^{(1)}(y) &= \iiint dy'[y'-y]g_\tau(y'|y) \qquad (25) \\ &= \int dq \left(M_{p_\tau}^{(1)}(q) + [q-y]\right)\tilde{f}(q|y) \quad . \end{aligned}$$

For $\tau \ll 1$ one may use (21). Furthermore applying (24) provides a closed expression for the first moment:

$$\begin{aligned} M_{g_\tau}^{(1)}(y) &= \tau \int dq D^{(1)}(q)\tilde{f}(q|y) \qquad (26) \\ &\quad + \frac{\int dq[q-y]f(y|q)P(q)}{\int dx f(y|q)P(q)} \\ &= \tau \int dq D^{(1)}(q)\tilde{f}(q|y) + \gamma_1(\sigma, y) \end{aligned}$$

The second part of this expression is independent on the time increment τ. This contribution is responsible for a divergent behavior of the limit (4a).

3.3 Second Moment $M_{g_\tau}^{(2)}$

For the second moment one proceeds in an analogous manner:

$$\begin{aligned} M_{g_\tau}^{(2)}(y) &= \iiint dy'[y'-y]^2 g_\tau(y'|y) \qquad (27) \\ &= \int dq \left(2(q-y)M_{p_\tau}^{(1)}(q) + M_{p_\tau}^{(2)}(q)\right) \\ &\quad \times \tilde{f}(q|y) + \int dq[q-y]^2\tilde{f}(q|y) + \sigma^2 \end{aligned}$$

Again inserting the Itô taylor expansion for the moments yields:

$$\begin{aligned} M_{F_\tau}^{(2)}(y) &= 2\tau \int dq(q-y)D^{(1)}(q)\tilde{f}(q|y) \\ &\quad + \tau \int dq D^{(2)}(q)\tilde{f}(q|y) \\ &\quad + \gamma_2(\sigma, y) \end{aligned} \tag{28}$$

In this case one finds the offset

$$\gamma_2(\sigma, y) = \frac{\int dq[q-y]^2 f(y|q)P(q)}{\int dq f(y|q)P(q)} + \sigma^2 \quad . \tag{29}$$

3.4 Use for analysis of noisy data

Knowledge of the expressions (27) and (28) can be exploited for the analysis of noisy data. $M_{g_\tau}^{(n)}(y)$ can be calculated from time series data. This has to be done for several time increments τ enclosing the minimal increment determined by the sampling rate. If the sampling rate is sufficient high the slope as well as the offsets at $\tau \equiv 0$ can be extrapolated.

The main problem is to calculate an estimate for $D^{(1)}$ and $D^{(2)}$ from slopes and offsets of the moments. As the inverse pdf $\tilde{f}(q|y)$ is a function of the stationary distribution of the Langevin process, the particular equations for the slopes and offsets are coupled.

However, for simple low-parametric – like e.g. Ornstein-Uhlenbeck – processes these integrals can be solved analytically. This allows for determination of the model parameters as well as the strength of the external noise source from time series data.

For more complicated processes higher moments have to be taken under consideration.

4 Conclusion

Summarizing, we have outlined operational methods for the estimation of drift and diffusion terms from experimental time series of stochastic Langevin processes.

In contrast to previous approaches the algorithm presented in section 2 does not rely on conditional moments in the small time increment limit. Based on a first approximation an iterative refinement of the estimated stochastic process is performed by minimization of the Kullback-Leibler distance between estimated and measured two time probability distributions. Although the effort evidently increases with increasing dimensions of the stochastic processes under investigation the proposed algorithm seems to be feasible for at least a modest number of degrees of freedom.

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