Estimation of drift and diffusion coefficients from sparsely sampled time series data

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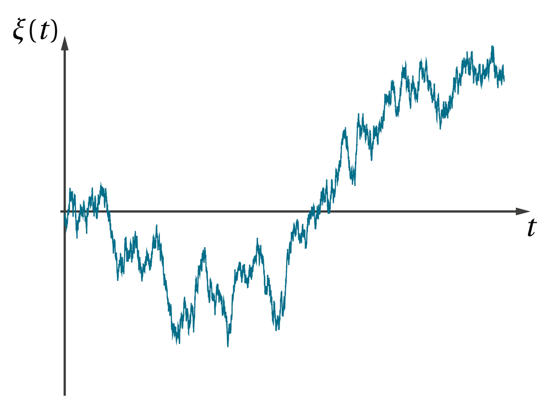
Abstract

We present a novel method to estimate drift and diffusion coefficients from data of stationary, univariate Markov processes via optimization [1]. The method takes advantage of a recently reported approach [2] that allows to calculate exact finite sampling interval effects by solving the adjoint Fokker-Planck equation. Therefore, it is well suited for the analysis of sparsely sampled time series. The optimization can be performed either making a parametric ansatz for drift and diffusion functions or also in a parameter free fashion. We present several numerical examples with synthetic time series that demonstrate the power of the method.

Langevin and Fokker-Planck description of complex systems

Given a data set of a stochastic time series



we try to find a model:

$$\dot{\xi}(t) = \underbrace{h(\xi(t),t)}_{\text{deterministic}} + \underbrace{g(\xi(t),t)\cdot\Gamma(t)}_{\text{stochastic}}$$

If

- noise is δ correlated: $\langle\Gamma(t)\Gamma(t')\rangle = \delta(t-t')$,
- and Gaussian distributed,

the process can be described by a Fokker-Planck equation

$$\frac{\partial}{\partial t}f_\xi(x,t) = \left[-\frac{\partial}{\partial x}\underbrace{D^{(1)}(x,t)}_{\text{drift}} + \frac{\partial^2}{\partial x^2}\underbrace{D^{(2)}(x,t)}_{\text{diffusion}}\right] f_\xi(x,t)\,,$$

with

- $f_\xi(x,t)$: probability density function of the process $\xi(t)$,
- $D^{(1)}(x,t) = h(x,t)$,
- $D^{(2)}(x,t) = \frac{1}{2}g^2(x,t)$.

Kramers-Moyal (KM) coefficients:

$$D^{(n)}(x) = \lim_{\tau\to 0}\frac{1}{n!\tau}\left\langle[\xi(t+\tau)-\xi(t)]^n\right\rangle\big|_{\xi(t)=x}$$

KM coefficients can, in principal, be estimated from time series data, see [3] for an overview.

Finite Time Effects

- Finite Time KM coefficients:

$$D_\tau^{(n)}(x) = \frac{1}{n!\tau}\left\langle[\xi(t+\tau)-\xi(t)]^n\right\rangle\big|_{\xi(t)=x}$$

- τ small enough $\Rightarrow D_\tau^{(n)}(x) \approx D^{(n)}(x)$
- $\tau_{\min}$ = Samplingintervall
- For larger τ, deviations become important, see [5, 6, 7].
- Exact finite time KM coefficients can be computed with a procedure introduced by Lade [2].
- In this work, Lade's method was inverted to obtain the true KM coefficients from measured finite time coefficients via optimization.

Lade's method

Finite time coefficients [6]:

$$D_\tau^{(n)}(x) = \frac{1}{n!\tau}M_\tau^{(n)}(x) = \frac{1}{n!\tau}\left\langle[\xi_{t+\tau}-\xi_t]^n\right\rangle\big|_{\xi_t=x} \qquad (1)$$

$$\begin{aligned} M_\tau^{(n)}(x) &= \int_{-\infty}^{\infty}(y-x)^n p_\xi(y,t+\tau|x,t)\,\mathrm{d}y \\ &= \int_{-\infty}^{\infty}(y-x)^n e^{\hat{L}(y)\tau}\delta(y-x)\,\mathrm{d}y \\ &= e^{\hat{L}^\dagger(y)\tau}(y-x)^n\big|_{y=x} \end{aligned}$$

Adjoint Fokker-Planck operator:

$$\hat{L}^\dagger(x) = D^{(1)}(x)\frac{\partial}{\partial x} + D^{(2)}(x)\frac{\partial^2}{\partial x^2}$$

Lade's interpretation [2]:

$$\frac{\partial W_{n,x}(y,t)}{\partial t} = \hat{L}^\dagger(y)W_{n,x}(y,t) \qquad (2)$$

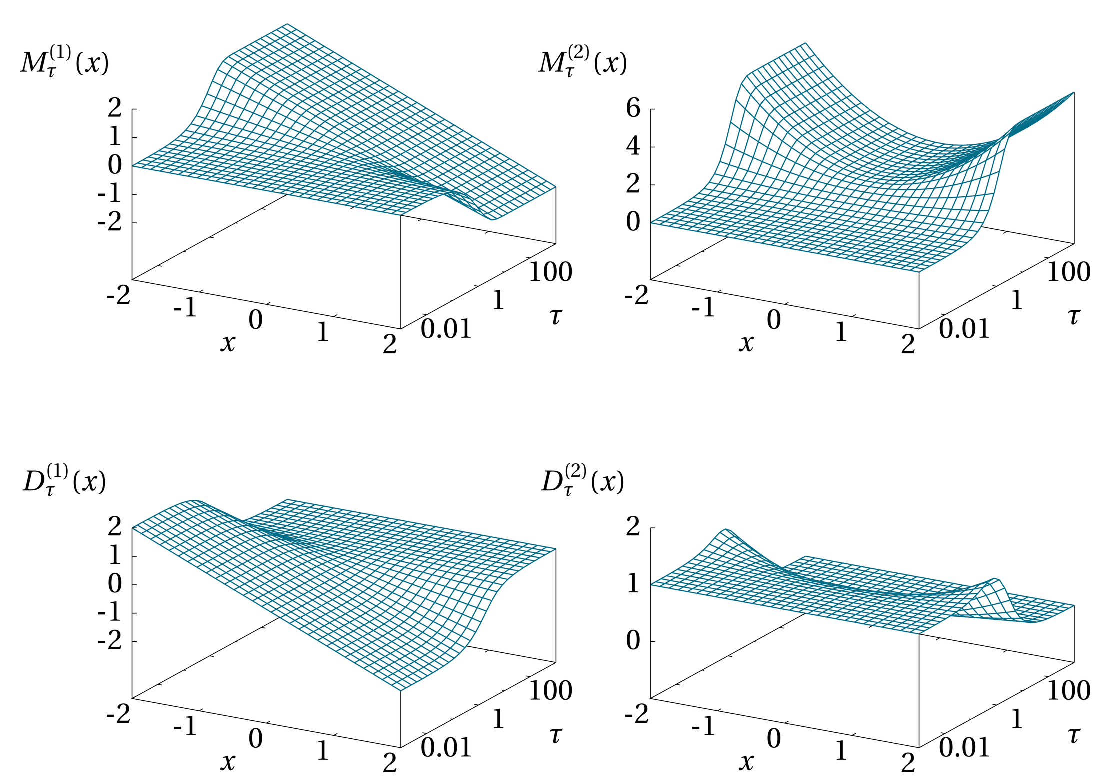
$$W_{n,x}(y,0) = (y-x)^n \qquad (3)$$

$$\Rightarrow \boxed{M_\tau^{(n)}(x) = W_{n,x}(y=x,t=\tau)}$$

Given $D^{(1)}(x)$ and $D^{(2)}(x)$, $D_\tau^{(n)}(x)$ can be calculated by integrating the corresponding adjoint FPE, Eq. (2), with initial condition (3) up to time τ.

Example of finite time effects

Ornstein-Uhlenbeck process:



The figure shows the finite time drift and diffusion (lower panels) and the corresponding conditional moments (upper panels) for an Ornstein-Uhlenbeck process with $D^{(1)}(x) = -x$ and $D^{(2)}(x) = 1$. As one can clearly see, the correlation time $\tau_c = 1$ seperates two different regimes. In the regime $\tau \ll \tau_c$, the finite time KM coefficients have converged to the true coefficients. Finite time effects can be safely neglected in this case. In the regime $\tau \gg \tau_c$, the first conditional moment becomes linear in x and the second moment becomes quadratic. Both moments become constant with respect to τ. The corresponding KM coefficients have the same dependence on x but, according to Eq. (1), decay to zero with τ^{-1}.

Limit of statistical independence [7, 8]

$$D_\tau^{(n)}(x) = \frac{1}{n!\tau}\left\langle[\xi_{t+\tau}-\xi_t]^n\right\rangle\big|_{\xi_t=x} := \frac{1}{n!\tau}M_\tau^{(n)}(x)$$

$$\begin{aligned} M_\tau^{(n)}(x) &= \int_{-\infty}^{\infty}(y-x)^n p_\xi(y,t+\tau|x,t)\,\mathrm{d}y \\ &\overset{\tau\gg\tau_c}{\longrightarrow} \int_{-\infty}^{\infty}(y-x)^n f_\xi(y)\,\mathrm{d}y \end{aligned}$$

$$M_\tau^{(1)}(x) \to \langle\xi\rangle - x$$

$$M_\tau^{(2)}(x) \to \langle\xi^2\rangle - 2\langle\xi\rangle x + x^2$$

$$D_\tau^{(1)}(x) \to \frac{1}{\tau}[\langle\xi\rangle - x]$$

$$D_\tau^{(2)}(x) \to \frac{1}{2\tau}\left[\langle\xi^2\rangle - 2\langle\xi\rangle x + x^2\right]$$

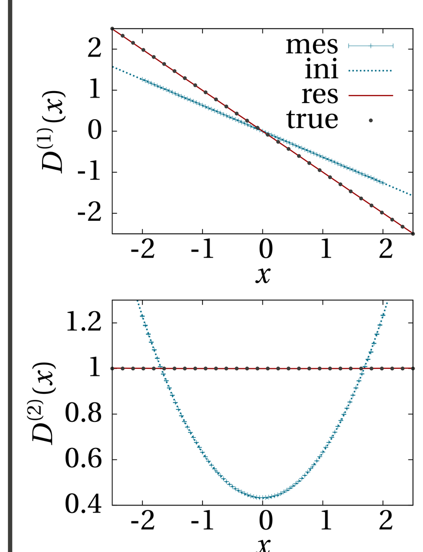
Outline of the method

- Estimate the conditional moments $\hat{M}_{\tau_i}^{(1,2)}(x_j)$ and the corresponding statistical errors $\hat{\sigma}_{ij}^{(1,2)}$ for $\tau_1,\ldots,\tau_M$ and $x_1,\ldots,x_N$ from time series data with the method described in [4].
- Make a parametric ansatz for $D^{(1,2)}(x,\sigma)$.
- Solve the corresponding adjoint FPE which yields $M_{\tau_i}^{(1,2)}(x_j,\sigma)$.
- Obtain the correct parameters σ by minimizing the least square potential

$$V(\sigma) = \sum_{i=1}^{M}\sum_{j=1}^{N}\left[\frac{\left\{\hat{M}_{\tau_i}^{(1)}(x_j) - M_{\tau_i}^{(1)}(x_j,\sigma)\right\}^2}{\left(\hat{\sigma}_{ij}^{(1)}\right)^2} + \frac{\left\{\hat{M}_{\tau_i}^{(2)}(x_j) - M_{\tau_i}^{(2)}(x_j,\sigma)\right\}^2}{\left(\hat{\sigma}_{ij}^{(2)}\right)^2}\right]$$

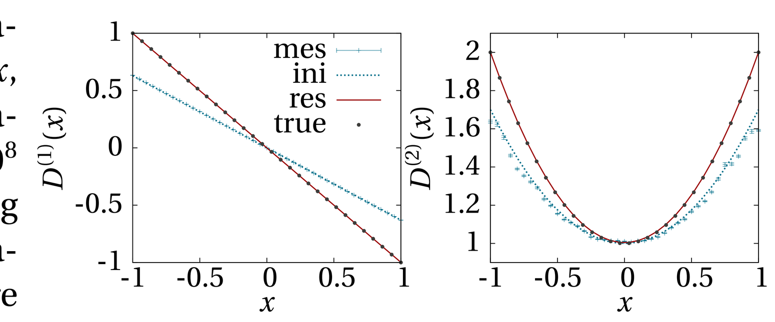
- Regarding the optimization, a trust region algorithm yields good performance.

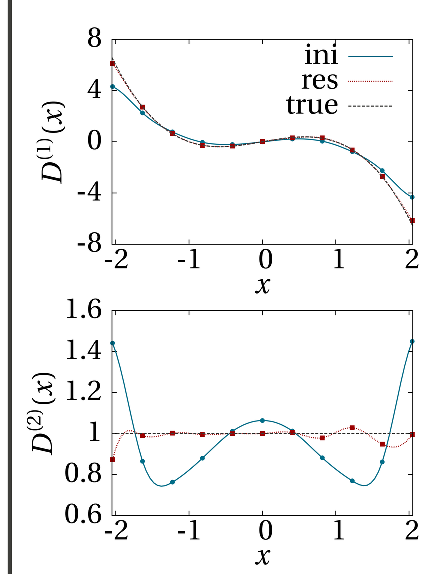
Numerical examples



Results for an Ornstein-Uhlenbeck process with $D^{(1)}(x) = -x$, $D^{(2)}(x) = 1$. The analyzed time series consists of 10^7 data points with a sampling interval $\tau_1 = 1$. The blue crosses with error bars are the estimated finite time coefficients $D_{\tau_1}^{(1)}$ (top) and $D_{\tau_1}^{(2)}$ (bottom). The blue dotted curves show the initial guess for the optimization, and the red solid ones show the result. For comparison, the true coefficients are also plotted (black dots).

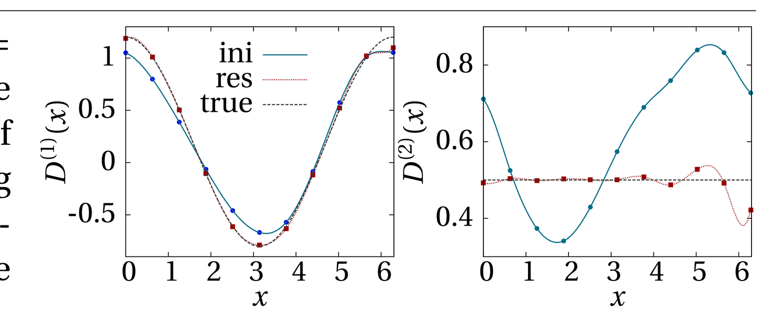
System with multiplicative noise: $D^{(1)}(x) = -x$, $D^{(2)}(x) = 1 + x^2$. The analyzed time series consists of 10^8 data points with a sampling interval $\tau_1 = 1$. The representation is analogous to the figure above.





Bistable system with $D^{(1)}(x) = x - x^3$, $D^{(2)}(x) = 1$. The analyzed time series consists of 10^7 data points with a sampling interval $\tau_1 = 0.1$. The blue and red symbols are sampling points, from which the corresponding curves (blue solid and red dotted lines) are computed as spline interpolations, and serve as optimization parameters. The blue dots represent the initial condition derived from the finite time coefficients $D_{\tau_1}^{(1,2)}$. The red squares show the result of the optimization. The black dashed curves show the true coefficients for comparison.

Phase dynamics with $D^{(1)}(x) = 0.2 + \cos(x)$, $D^{(2)}(x) = 0.5$. The analyzed time series consists of 10^7 data points with a sampling interval $\tau_1 = 1$. The representation is analogous to the figure above.



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